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Sn-modification of Pt₇/alumina model catalysts: Suppression of carbon deposition and enhanced thermal stability

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ABSTRACT

An atomic layer deposition process is used to modify size-selected Pt₇/alumina model catalysts by Sn addition, both before and after Pt₇ cluster deposition. Surface science methods are used to probe the effects of Sn-modification on the electronic properties, reactivity, and morphology of the clusters. Sn addition, either before or after cluster deposition, is found to strongly affect the binding properties of a model alkene, ethylene, changing the number and type of binding sites, and suppressing decomposition leading to carbon deposition and poisoning of the catalyst. Density functional theory on a model system, Pt₄Sn₃/alumina, shows that the Sn and Pt atoms are mixed, forming alloy clusters with substantial electron transfer from Sn to Pt. The presence of Sn also makes all the thermally accessible structures closed shell, such that ethylene binds only by π -bonding to a single Pt atom. The Sn-modified catalysts are quite stable in repeated ethylene temperature programmed reaction experiments, suggesting that the presence of Sn also reduces the tendency of the sub-nano clusters to undergo thermal sintering.

I. INTRODUCTION

Catalyst deactivation by coking, i.e., carbon deposition, is a significant problem in many catalysis applications at high temperature under hydrocarbon-rich conditions, such as dehydrogenation of alkanes to alkenes¹⁻³ for petroleum processing, including applications based on Pt nanoparticle catalysts.⁴⁻⁹ In industrial applications, it is possible to regenerate catalysts by periodically oxidizing the coke away at high temperatures; however, for nano-catalysts, the high regeneration temperatures can lead to sintering and loss of activity. Sub-nano clusters have most or all of the catalytic metal in the reactant-accessible surface layer, thus improving the use of precious metals. However, such small clusters are less thermodynamically stable than larger particles, thus sintering is even more of a problem. One application of interest is the use of alkane-to-alkene dehydrogenation in hot hydrocarbon fuels as an endothermic reaction to cool air vehicle fuel systems at high temperatures, the problem being that dehydrogenation of the alkene product creates coke precursors. Coking is a particular problem because it can lead to clogging of small channels or injectors, and regeneration may not be a practical option. One strategy for sintering prevention is to stabilize the catalyst by forming porous silica or alumina coating over the nanoparticle catalysts;¹⁰⁻¹³ however, despite achieving anti-sintering effects, this can also block the catalytic sites.¹⁴

Previous research on Pt bimetallic catalysts introduced elements such as tin, nickel, cobalt, copper, and germanium into the nanoparticle catalysts¹⁵⁻²². The role of these second elements is to alter the geometric and electronic properties of Pt particles to improve the stability of the catalyst and selectivity of catalytic reactions. Among these elements, Sn has been widely investigated, and PtSn bimetallic catalysts showed favorable selectivity and low activity loss, especially toward light alkene production^{1, 23-26}.

For example, Koel and co-workers reported UHV studies of ordered PtSn surface alloys formed by depositing Sn on Pt (111) single crystals. In particular, they found that Sn-alloying suppressed dehydrogenation of adsorbed ethylene and other alkenes such as propylene and isobutylene, thus reducing formation of coke precursors.^{27, 28} The temperature-programmed desorption (TPD) results showed that as the Sn coverage increased, the binding energies of the alkenes to the surface decreased substantially, resulting in desorption temperatures dropping by ~100 K in the case of ethylene. As a result, H₂ desorption, signaling ethylene decomposition and coking, was almost completely suppressed. These changes in binding energy and desorption behavior occurred despite the observation that Sn alloying had no effect on low temperature sticking probability, nor on the saturation alkene coverage. It was proposed that ethylene binds in a di- σ geometry on both the Pt and PtSn alloy surfaces.

Recently, Hook et al. used density functional theory (DFT) to examine ethane dehydrogenation over PtSn surface alloys, finding, consistent with the experiments of Koel and co-workers, that Sn depresses the alkene desorption energy below the barrier for dehydrogenation, due to a combination of geometric and electronic effects.²⁹ Ethylene was found to bind in a di- σ fashion on both the Pt and PtSn alloy surfaces. The results were in line with an earlier DFT study by Yang et al. of propane dehydrogenation, where formation of coke precursors was also predicted to be suppressed by Sn alloying due to lowering of the propylene desorption energy below the barrier for further dehydrogenation.³⁰

Dumesic and co-workers used microcalorimetric and IR spectroscopy methods to study ethylene interactions with Pt/SiO₂ and several different stoichiometry PtSn/SiO₂ catalysts with metal particle sizes in the 2 to 5 nm range.^{31, 32} On Pt/SiO₂, both di- σ and π -bonded ethylene were observed. Sn alloying reduced the heat of adsorption of ethylene on the catalysts, and with

increasing Sn content, the fraction of π -bonded ethylene increased, thus differing from the results on extended PtSn surface alloys. As shown below, moving to sub-nanometer clusters introduces additional differences.

We have been using a combination of experiments and density functional theory (DFT) to probe methods to mitigate coking and sintering of sub-nano, size-selected model Pt_n/alumina catalysts. Ethylene temperature-programmed desorption (TPD), along with surface probes such as low energy ion scattering (ISS) and X-ray photoelectron spectroscopy (XPS) is used to test the propensity toward coking and sintering. Monitoring the branching between desorption and dehydrogenation, which deposits carbon, provides a signature of coking, and observing the evolution of the catalyst morphology and adsorption properties during multiple TPD runs, provides insight into thermal processes. Pure Pt_n/alumina catalysts were found to deactivate rapidly in sequential ethylene TPD experiments, primarily due to the deposition of carbon on the clusters.³³ We showed that diborane could be used to selectively borate size-selected Pt_n seed clusters on the alumina support,³⁴ thus generating clusters anchored to the support by Pt-B-O bonds, and modifying the electronic properties such that dehydrogenation and carbon deposition were almost completely suppressed.³⁵

The success of coking prevention was attributed to boration substantially reducing the ethylene binding energy, so that desorption occurred in preference to dehydrogenation. DFT showed that the PtB clusters support only weak π -interaction with ethylene, favoring ethylene desorption, whereas pure Pt clusters can also bind ethylene in a strong di- σ fashion, activating it for dehydrogenation. Importantly, this property was observed for the entire thermally-accessible ensemble of cluster isomers, assessed via global optimization and Boltzmann statistics.^{36, 37} A concern regarding boration, however, is that because it substantially weakens the alkene (i.e.,

ethylene) binding to the clusters, it might also increase the activation barriers for the desired alkane-to-alkene conversion.

Recently we developed an atomic layer deposition (ALD) approach that allows Sn to be selectively deposited on size-selected Pt_n clusters on oxide thin film supports. The clusters act as seeds to initiate the ALD process, thus Sn_mPt_n clusters of well-defined size and stoichiometry can be prepared.³⁸ For Pt_n on SiO_2 the Sn deposition process was highly selective, depositing Sn on Pt cluster sites at least 50 times more efficiently than on the SiO_2 support sites. Here we apply this Sn deposition method to modifying model Pt_n /alumina catalysts and examining the effects on ethylene binding and suppression of carbon deposition. Alumina was chosen for the initial catalysis study of Pt_nSn_m clusters, to allow comparisons with the Pt_n /alumina and Pt_nB_m /alumina systems, where detailed experimental and DFT results are available.

The resulting model Sn-Pt catalysts are studied using *in situ* surface chemistry methods to characterize their stoichiometries, electronic properties, morphology, and activity for ethylene binding and dehydrogenation. DFT is used to model the structures, energetics, electronic properties of both model SnPt supported clusters, and binding of ethylene to the clusters. Finally, we compare the effects of Sn-modifying the support, prior to deposition of the size-selected Pt_7 clusters, vs. modifying the samples after Pt_7 deposition. We focus the experimental work here on Pt_7 because this was identified as a particular active cluster size for Pt_n /alumina, and also coked/deactivated rapidly. The DFT work focused on a smaller, more tractable size: Pt_4Sn_3 /alumina.

METHODOLOGY

Experimental Methodology

The instrument used in the experiments has been described previously.^{33, 34, 39} Briefly, a laser vaporization/supersonic expansion source was used to produce Pt_n^+ clusters that were collected by a set of quadrupole ion guides, mass-selected by a quadrupole mass filter, and then guided by a final quadrupole into the ultrahigh vacuum (UHV) system (1.5×10^{-10} Torr), where they were deposited on a planar alumina support to form a model catalyst. The support is mounted via heater wires to a cryostat, and its temperature can be controlled between 120 K and 2100 K.

The alumina support was a thin film grown on a Ta (110) single crystal by the following procedure. The Ta single crystal was cooled below 130 K and then annealed to 2100 K for 5 minutes to desorb Pt and Al_2O_3 from the previous experiment, with the cleanliness checked by X-ray photoelectron spectroscopy (XPS). The Ta crystal was then transferred to a UHV antechamber, where Al was evaporated onto it in 5×10^{-6} Torr of O_2 , maintaining the crystal at 970 K. According to Chen and Goodman,⁴⁰ thin films of alumina grown on Ta(110) by this method have a distorted hexagonal lattice similar to the (0001) face of α -alumina or (111) face of γ -alumina. The film thickness was determined by modeling⁴¹ the measured Al/Ta XPS ratio using photoemission cross sections and asymmetry parameters from Yeh and Lindau⁴², and electron effective attenuation lengths (EALs) calculated with the database program of Powell and Jablonski.⁴³ Thicknesses were in the range from 4.7 to 5.7 nm, which we previously found to be thick enough to give thickness-independent chemistry for supported catalyst clusters, but thin enough to avoid charging during deposition or XPS.

For cluster deposition, the Al_2O_3 support was positioned just behind a 2 mm diameter exposure mask and then flashed to 700 K to remove adventitious adsorbates. As the sample cooled,

Pt_n^+ deposition was started as the sample temperature reached 300 K, with the coverage monitored via the neutralization current. The deposition continued as the sample cooled to 120 K and was terminated when the coverage reached 1.5×10^{14} Pt atoms/cm², corresponding to ~0.1 of a close-packed Pt monolayer (0.1 ML). In these experiments with Pt₇ clusters, 2.15×10^{13} clusters were deposited *per* cm².

Sn was incorporated into the samples using an ALD process developed by Gorey *et al.*³⁸ to prepare Pt_nSn_m alloy clusters on silica supports. Here, a freshly deposited Pt₇/Al₂O₃ sample was transferred into the UHV antechamber, then exposed to H₂ (6000 L), followed by SnCl₄ (24 L), followed by a final H₂ dose (6000 L), all at a sample temperature of 300 K. Gorey *et al.* showed that H selectively adsorbed on Pt atoms in the clusters, and that SnCl₄ preferentially reacted with hydrogenated Pt sites, losing HCl_(g) and binding SnCl_x to the clusters. During the second H₂ dose, additional HCl desorbed, leaving <10% of the Cl originally associated with the adsorbed Sn on the surface. This remaining Cl was desorbed as HCl by flashing the samples to 700 K. For consistency with the Gorey nomenclature, the sequence of gas exposures will be referred to as the “full treatment”, i.e., a Pt₇/alumina sample thus treated will be denoted FT/Pt₇/Al₂O₃. After heating, such a sample would be denoted heat/FT/Pt₇/Al₂O₃. For comparison, samples were also prepared by first exposing a freshly grown alumina-Ta(110) substrate to the full H₂/SnCl₄/H₂ treatment, then heating the substrate, then depositing 0.1 ML of Pt₇. These samples will be referred to as Pt₇/heat/FT/Al₂O₃. Finally, control experiments were done on Pt-free alumina given the full treatment, and these are denoted FT/Al₂O₃. Mg K α XPS was used to quantify the amount of Sn deposited on the samples. Samples were characterized as-deposited and after being flashed to 700 K to desorb residual H and Cl.

Low energy He^+ scattering (ISS) was used to probe the surface morphology of the samples. A 0.2 μA He^+ beam impinged on the surface at 1 keV with a 45° angle of incidence and scattered He^+ was detected along the surface normal. The He^+ beam caused some sputtering and other sample damage, and, to avoid damaging effects, ISS was performed either at the end of other experiments or on separately prepared samples. To compensate for any run-to-run variations in the He^+ flux, the Pt and Sn ISS peak intensities were normalized to the total scattered He^+ intensity.

Adsorbate binding and reactivity of the samples were probed by temperature-programmed desorption (TPD). In the TPD experiments, the sample temperature was held at 150 K while it was dosed with 5 L of C_2D_4 . This dose temperature was chosen as being low enough to allow the cluster binding sites to be saturated while minimizing adsorption on the alumina support. After dosing, the sample was cooled to 130 K, and then ramped to 700 K at 3 K *per* second. During the heat ramp, molecules desorbing from the surface were monitored by a differentially pumped mass spectrometer that views the sample through the ~ 3 mm aperture in a skimmer cone. The ion signals are used to estimate the number of neutral molecules of each type desorbing from the sample, using a calibration procedure discussed elsewhere, and described in more detail in the SI. The absolute uncertainty of the resulting desorption numbers is estimated to be 50%.

Computational Methodology

Calculations were performed as discussed in previous work³⁴. Projector-augmented wave method⁴⁴ and PBE functional⁴⁵ were used within the Vienna ab initio simulation package (VASP).⁴⁶⁻⁴⁹ Plane-wave kinetic energy cut-off of 400.0 eV and convergence criteria of 10^{-6} eV for electronic (SCF) steps were employed. Note that the bottom half of the slab was kept fixed during the relaxation. Geometric relaxation was performed until forces on each atom were smaller than 0.01 eV/Å. In addition, Gaussian smearing with the sigma value of 0.1 eV was used. The

hexagonal symmetry alumina thin film used in the experiments was modeled computationally as an α -alumina (0001) surface. The cell parameters of $a = 4.807 \text{ \AA}$ and $c = 13.126 \text{ \AA}$ were obtained by optimizing the bulk structure with stringent electronic and geometric convergence criteria, the details of which can be found here.³³ Moreover, the slab was modeled as a (3×3) unit cell with a vacuum gap of 15 \AA . Since a fairly large super cell was used in this study, a k-point grid of $1 \times 1 \times 1$ centered at the Γ -point was instituted.

In order to produce initial geometries for clusters on the Al_2O_3 surface, we used our in-house parallel global optimization and pathway toolkit (PGOPT), which automatically generates initial structures based on the bond length distribution algorithm (BLDA).⁵⁰ Each structure was optimized with DFT, and duplicates were filtered out thereafter. Finally, partial charges on each atom in the cluster were obtained using the Bader charge scheme.⁵¹⁻⁵⁴

RESULTS AND DISCUSSION

A. XPS

Mg K α XPS studies of these samples were done over a period when the spectrometer sensitivity varied significantly due to aging of the electron detector, thus the raw intensities must be corrected to allow sample-to-sample comparisons. If our alumina film supports were more than ~ 3 times thicker than the Al 2p electron effective attenuation length (EAL), the intensity of the Al 2p peak would be independent of film thickness, and the Pt and Sn intensities could be corrected by simply normalizing them to the Al 2p intensities. The Al 2p EAL in alumina, calculated using the database program of Powell and Jablonski,⁴³ is 2.1 nm , while our alumina films had thicknesses varying from 4.7 to 5.7 nm – not quite thick enough to give thickness-independent Al 2p signal.

Therefore, the sensitivity correction must be done in two steps, as summarized in Table S1:

1. The film thickness for each sample was determined from the Al/Ta XPS ratio as described above, and then the EAL was used to correct the measured Al 2p intensities to what they would have been if all the samples had films with identical thickness, chosen as 4.7 nm because several of the samples did have this thickness.
2. The thickness-corrected Al 2p intensities were then used to calculate the factors needed to correct for the declining sensitivity of the electron detector, and these factors (last column, Table S1) were then used to scale the Pt and Sn intensities in Fig. 1.

The assumption in this correction process is that the Al 2p intensities are unaffected by the deposition of Pt and/or Sn on the alumina films. Given that the Pt and Sn coverages are small, on the order of 0.1 ML, any attenuation of Al 2p signal should be in the few percent range, and the resulting error is within the uncertainties due to low XPS signal level for Pt and Sn, which we estimate to be $\pm 15\%$ for Pt, and $\pm 5\%$ for Sn.

The background-subtracted and sensitivity-corrected XPS results for all the samples are shown in Fig. 1, along with the fits used to extract the integrated intensities. The integrated intensities and intensity ratios are given in Table 1, and the binding energies (BEs) for the Pt 4d_{5/2} and Sn 3d_{5/2} peaks are in Table S2.

The left column of Fig. 1 shows the Pt 4d XPS for all the samples. The first point to note is that the intensities are similar, as expected, because all samples had identical coverages of Pt₇. Some variation in the Pt intensity is expected because different samples have Sn deposited on top of the Pt, or have been heated which may change the cluster structure. Therefore, the attenuation of Pt photoelectrons should vary from sample to sample. Note that the Pt intensities are quite low, because the Pt coverage is low, and also because we monitored the Pt 4d XPS, rather than the more

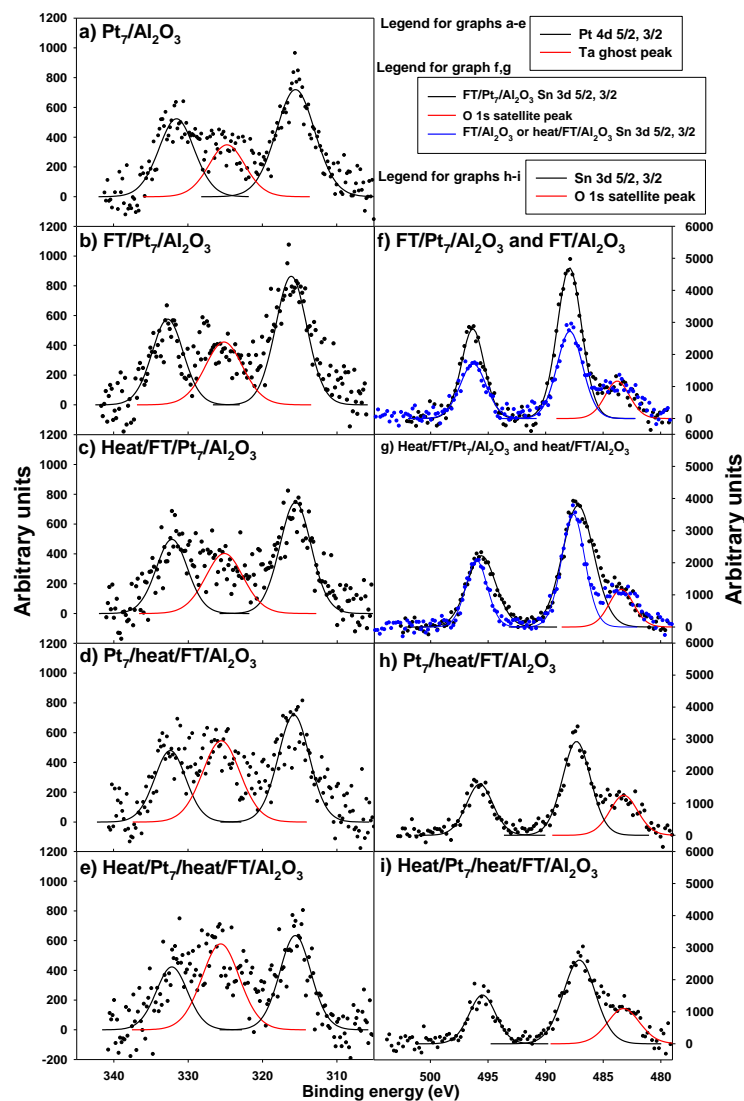


Figure 1. Left column: Pt 4d XPS region spectra. Peaks for Pt 4d_{5/2} and 4d_{3/2} are indicated with black fitted curves, the red curve indicates a Ta 4s ghost peak. Right column: Sn 3d XPS region. Peaks for Sn 3d_{5/2} and 3d_{3/2} are indicated with black or blue curves. The red curve indicates an Mg K β O 1s satellite peak. “FT” refers to the full H₂/SnCl₄/H₂ treatment.

intense 4f since the 4f has substantial interference from Al 2p. As a result, the estimated uncertainties in the corrected integrated Pt intensities given in Table 1 are $\sim \pm 15\%$.

As shown in Table S2, the Pt 4d_{5/2} BE for Pt₇/Al₂O₃ is 315.4 eV, compared to 314.6 eV for bulk Pt.⁵⁵ This 0.8 eV shift to higher BE is attributed to the effects of the small cluster size on stabilization of the photoemission final state.^{56, 57} After the full Sn deposition treatment, and before heating (FT/Pt₇/Al₂O₃), the Pt 4d BE is shifted to 316.2 eV, presumably due to the combined effects of adsorbed Sn, Cl, and H, which may affect both the Pt oxidation state, and the final state stabilization. After heating to drive off H and Cl, the BE dropped back to 315.5 eV. When the alumina support was given the full Sn treatment and heated prior to Pt₇ deposition, the Pt 4d BE was 315.7 eV, and after heating to 700 K, the BE also dropped back to 315.5 eV.

The Sn XPS provides insight into both the amount of Sn present and its chemical state. First, consider the unheated samples. Fig. 1f compares the Sn XPS for the FT/Al₂O₃ and FT/Pt₇/Al₂O₃ samples. By the integrated Sn intensities (Table 1), a substantial Sn signal is observed in the absence of Pt₇, but that signal increases by a factor of ~1.6 when Pt₇ is present. Given that the Pt₇ is present at only 0.1 ML coverage, this implies that Sn deposition is roughly 6 times more efficient on Pt sites, compared to alumina sites. In comparison to Sn deposition by the same process on Pt_n/SiO₂, the selectivity is lower here, largely because the SiO₂ was much more inert toward the H₂/SnCl₄/H₂ treatment process. The intensities are analyzed below to extract numbers of Sn atoms deposited.

Table 1. Corrected intensities of Sn 3d, Pt 4d, Al 2s and values of their ratios. “FT” refers to the full H₂/SnCl₄/H₂ treatment. The bold font highlights the Sn and Pt to Al ratios.

	Al ₂ O ₃ thickness (nm)	corrected intensities					
		Sn	Pt	Al	Sn/Al	Pt/Al	Sn/Pt
Pt₇/ Al₂O₃	5.3		8051	54972	0.15		
FT/Al₂O₃	5.2	12771		54972	0.23		
Heat/FT/Al₂O₃	5.2	14074		54972	0.26		
FT/Pt₇/Al₂O₃	5.7	20006	7812	54972	0.36	0.14	2.56
Heat/FT/Pt₇/Al₂O₃	5.7	20413	6741	54972	0.37	0.12	3.03
Pt₇/heat/FT/Al₂O₃	4.7	13889	6505	54972	0.25	0.12	2.14
Heat/Pt₇/heat/FT/Al₂O₃	4.7	13865	5735	54972	0.25	0.10	2.42
Pt₇/heat/FT/Al₂O₃ post 6 TPDs	4.7	14841	5889	54972	0.27	0.11	2.52

After heating, the Sn intensity for FT/Al₂O₃ increased by ~10%, suggesting that the Cl and H present after the full treatment were attenuating the Sn signal, and demonstrating no significant Sn desorption occurring at 700 K. For the FT/Pt₇/Al₂O₃ sample, the Sn intensity also increased, but only by ~2%. The smaller increase suggests that the post-heating Sn binding geometry is such that there is still some attenuation of the Sn signal, as might occur if some Sn is alloyed with the Pt so that it is not in the surface layer. The ISS and theory discussed below address this point.

For Pt₇/heat/FT/Al₂O₃ sample, we might expect that the Sn intensity should be similar to that of the Ft/Al₂O₃ sample since the Sn treatment was applied to Pt-free alumina in both cases. The intensity was actually ~10% higher. Note, however, that the alumina film thicknesses were ~0.5 nm different in the two samples, which may influence Sn deposition. After heating, the Sn intensity for the heat/Pt₇/heat/FT/Al₂O₃ sample was essentially unchanged.

The Sn 3d_{5/2} peak for FT/Pt₇/Al₂O₃ is broadened and shifted to lower binding energies at 487.9 eV, when Pt₇ was present, and also at 487.9 eV for FT/Al₂O₃. For the samples prepared by Sn deposition on alumina and heating, prior to Pt₇ deposition, the Sn BEs are shifted to lower energy (487.1 to 487.3 eV), but in all cases, the BEs are substantially higher compared that the BE

reported for Sn bulk metal (~485 eV), and closer to the values reported for various oxygenated or halogenated Sn compounds (up to ~488 eV).⁵⁵ The high Sn binding energies, thus, suggest that Sn is in an oxidized state on the samples. DFT results regarding this question are presented below.

The Sn/Pt stoichiometry of the samples can be determined from the corrected integrated intensity ratios in Table 1. For samples containing 0.1 ML of Pt in the form of Pt₇, we can use the Sn/Pt

ratio, along with Pt 4d and Sn 3d photoemission cross sections (σ_{Sn} ,

σ_{Pt}), obtained from the work of Yeh

and Lindau.⁴² Taking advantage of

the fact that both Pt and Sn are present only in the surface of the

sample, and assuming the attenuation of the associated

photoelectrons is negligible, the

Sn/Pt coverage ratio ($X_{\text{Sn}}/X_{\text{Pt}}$) is

related to the XPS intensity ratio ($I_{\text{Sn}}/I_{\text{Pt}}$) by the following relation:

$$X_{\text{Sn}}/X_{\text{Pt}} = (I_{\text{Sn}}/\sigma_{\text{Sn}})/(I_{\text{Pt}}/\sigma_{\text{Pt}}) \quad (1)$$

The coverage of Pt-free samples can be estimated by comparison of the Sn intensities for the Pt₇-containing and Pt-free samples, and the results are summarized in Table 2.

For the FT/Al₂O₃ sample, the Sn intensity before heating gives an estimated Sn coverage of 15.0 Sn atoms *per* 10 nm² of the Al₂O₃ substrate, or 1.5×10^{14} Sn/cm², however, at this stage the Sn is still covered with adsorbed Cl (and possibly H), which attenuates the XPS. After heating to desorb these species, the Sn XPS intensity increased by ~10%, leading to an estimate of the Sn coverage

Table 2. The ratio of the number of Sn atoms to Pt atoms and the number of Sn atoms per 10 nm². “FT” refers to the full H₂/SnCl₄/H₂ treatment.

	Sn atoms/Pt atoms	Sn atoms/10 nm ²
FT/Al ₂ O ₃		15.0
Heat/FT/Al ₂ O ₃		16.5
FT/Pt ₇ /Al ₂ O ₃	1.62	24.3
Heat/FT/Pt ₇ /Al ₂ O ₃	1.65	24.8
Sn bound to Pt from FT/Pt ₇ /Al ₂ O ₃ and heat/FT/Pt ₇ /Al ₂ O ₃	0.55	8.3
Pt ₇ /Heat/FT/Al ₂ O ₃	1.09	16.4
Heat/Pt ₇ /Heat/FT/Al ₂ O ₃	1.09	16.4

of 16.5 Sn/10 nm², or 1.65×10^{14} Sn atoms/cm². This is comparable to the amount of Pt deposited in the Pt₇-containing samples, 1.5×10^{14} Pt atoms/cm², i.e., the non-selective Sn deposition on the alumina film gives coverage comparable to the Pt coverage in the cluster-containing samples. Sn deposition by the same approach on SiO₂ substrates was found to deposit only 3.5 Sn atoms/10 nm², i.e., roughly 1/5th the number on the alumina support. We attribute the much larger amount of non-selective Sn deposition on alumina to a larger density of defects or other sites capable of supporting Sn deposition.

When Pt₇ is present on alumina, ~60% more Sn was deposited, and for the FT/Pt₇/Al₂O₃ sample, the Sn/Pt ratio was 1.62, corresponding to 24.3 Sn atoms and 15 Pt atoms/10 nm², and when that sample was heated, the Sn intensity increased ~2% (due to desorption of Cl and H), but the Pt decreased by ~10%. No Pt desorption is observed, and thus, we attribute the decrease to the effects of alloying the clusters with Sn, which may include both the Sn atoms initially deposited on the Pt clusters, as well as Sn initially deposited on the alumina, that diffuses and binds to the clusters when the samples were heated. The ISS experiments, below, provide additional insight into this point. The increase in the Sn XPS intensity after heating implies 24.8 Sn atoms/10 nm², and if we assume that the Pt coverage is unchanged, then the Sn/Pt ratio after heating is 1.65.

The question is how many of the 24.8 Sn/10 nm² were deposited directly on the clusters, and how many become associated with the clusters after heating, as opposed to binding at defects on the alumina support. We can estimate the number of Sn depositing on clusters by assuming that the presence of 0.1 ML of Pt₇ on the surface does not affect the deposition of Sn on the surrounding Al₂O₃. In that limit, we can estimate that $24.8 - 16.5 = 8.3$ additional Sn atoms *per* 10 nm² deposited in association with the Pt₇ clusters, corresponding to 0.55 Sn/Pt atom, or ~4 Sn atoms/Pt₇ cluster. To the extent that the presence of Pt₇ blocks Sn deposition on the alumina, or captures Sn

initially impinging on the alumina, then the number of Sn atoms associated with the Pt₇ would be higher, up to 11.6 Sn/Pt₇ if all the Sn diffused and bound to the clusters. Note that, for the Pt_n/SiO₂ system, where little non-selective Sn deposition is observed on the SiO₂, the estimated Sn/Pt stoichiometry was ~6 Sn/Pt₇.

If similar analysis is applied to the Pt₇/heat/FT/alumina and heat/Pt₇/heat/FT/alumina samples, the conclusion is that the number of Sn depositing non-selectively on the alumina support was ~16 Sn atoms/10 nm², with essentially no difference between calculations based on the two spectra. The coverage of Pt₇ deposited on top of the Sn-modified surface is 2.14 Pt₇ clusters/10 nm², corresponding to 15 Pt atoms.

The important questions regarding these model catalysts are:

1. What effect does Sn modification have on the activity, selectivity, and stability of the catalysts?
2. Does Sn initially deposited on the alumina support migrate and bind to the Pt clusters, either as-deposited or when heated?
3. Is there a significant difference between the effects of Sn deposited initially on the alumina vs. on the Pt clusters?

TPD Results

Figure 2 summarizes the results of TPD experiments in which the Sn-modified model catalysts were saturated with C₂D₄ at 150 K, and then the numbers of desorbing C₂D₄ and D₂ molecules were monitored during 3 K/sec heat ramps to 700 K. A series of 6 TPD experiments was done for each sample, each preceded by a 150 K C₂D₄ dose. The calculated numbers of each type of molecule desorbing *per* cluster are tabulated in Table S3. For comparison, TPD data for Pt₇/Al₂O₃ measured under identical conditions by Baxter *et al.*³³ is plotted in the top row. Also

shown in each frame of the figure is the desorption observed from a Pt and Sn-free Al_2O_3 thin film sample.

As discussed in the Introduction, for our purposes, the interesting questions pertaining to the catalysis are: 1. How is the binding energy of C_2D_4 affected by the presence of Sn either on the clusters or the support? 2. How does Sn deposited on the clusters vs. on the support affect the branching to dehydrogenation? 3. In repeated TPD runs, how do the catalysts evolve, due to processes such as sintering or carbon deposition?

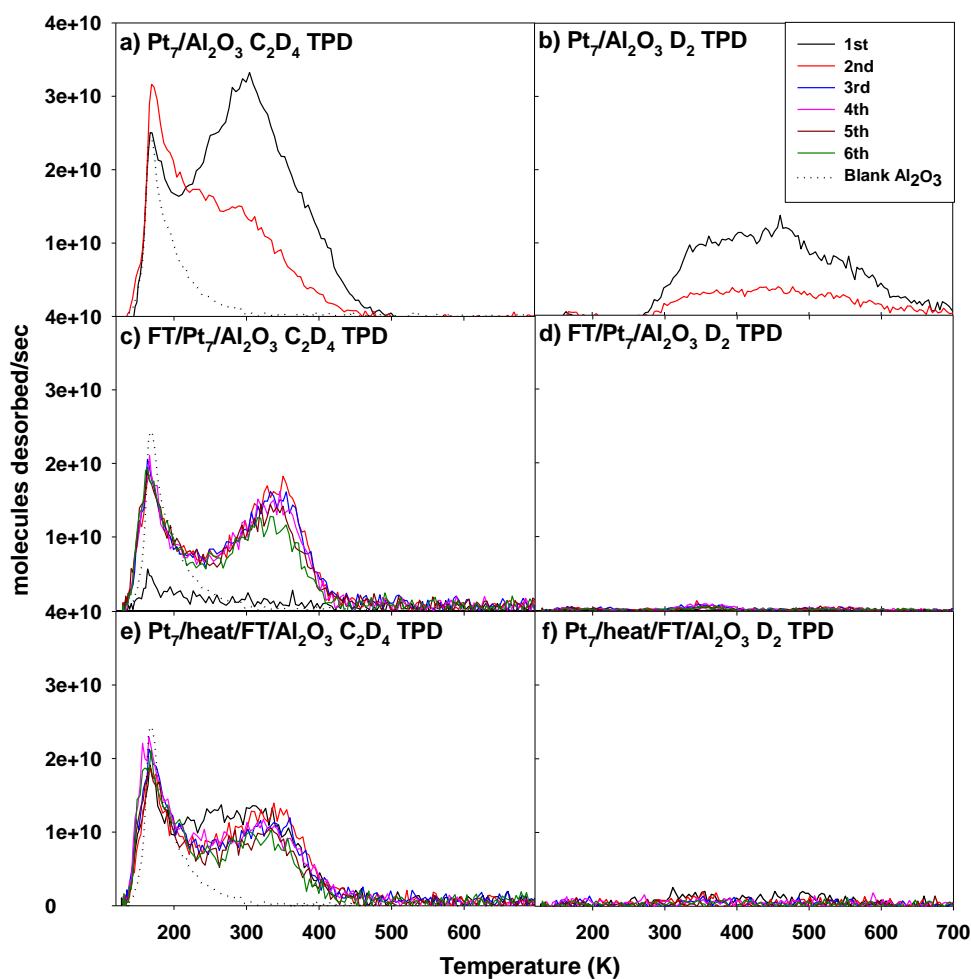


Figure 2. C_2D_4 and D_2 TPD data for the samples: a) $\text{Pt}_7/\text{Al}_2\text{O}_3$ C_2D_4 TPD, b) $\text{Pt}_7/\text{Al}_2\text{O}_3$ D_2 TPD, c) $\text{FT}/\text{Pt}_7/\text{Al}_2\text{O}_3$ C_2D_4 TPD, d) $\text{FT}/\text{Pt}_7/\text{Al}_2\text{O}_3$ D_2 TPD, e) $\text{Pt}_7/\text{heat}/\text{FT}/\text{Al}_2\text{O}_3$ C_2D_4 TPD, f) $\text{Pt}_7/\text{heat}/\text{FT}/\text{Al}_2\text{O}_3$ D_2 TPD. “FT” refers to the full $\text{H}_2/\text{SnCl}_4/\text{H}_2$ treatment.

It can be seen that for Sn-free Pt₇/Al₂O₃ (top row), the 1st TPD run has a low-temperature C₂D₄ desorption feature that matches that from the Al₂O₃ support, implying that this feature results from C₂D₄ desorbing from the support. Because the intensity of this peak is rather low, corresponding to only a small fraction of a monolayer of C₂D₄ desorbing, it is attributed to C₂D₄ bound at defects or other strong-binding sites on the surface.

There is also a higher temperature feature clearly associated with C₂D₄ desorbing from the Pt₇ clusters. No D₂ desorption is observed from the Al₂O₃ support, but in the 1st run on Pt₇/Al₂O₃, a large D₂ desorption feature is observed, implying that a significant fraction of the C₂D₄ undergoes dehydrogenation. We previously showed that no acetylene desorbs from this surface,³³ and thus, the D₂ signal is associated with carbon deposition – one C atom per D₂ molecule.

In the 2nd TPD run, the intensity of the Pt-associated C₂D₄ desorption decreased substantially, as did the amount of D₂ desorption. These changes were attributed mainly to the effects of the poisoning of cluster-associated binding sites by carbon deposition, observable by post-TPD C 1s XPS. Sintering probably also contributed to the deactivation process, although ISS and comparison of the effects of heating with and without C₂D₄,^{33,35} suggested that sintering during a single TPD run had only a modest effect for Pt₇ on the relatively defective Al₂O₃ thin film support. Only two TPD runs were reported in these experiments because the deactivation was so fast.

For the FT/Pt₇/Al₂O₃ sample, the 1st C₂D₄ TPD experiment was done on the unheated sample, and as shown in the 2nd row of the figure, little C₂D₄ desorption and no D₂ is observed. This implies that the Pt cluster sites were fully blocked by adsorbed H, Cl, and Sn and that many of the Al₂O₃ defect sites were also blocked, such that almost no C₂D₄ adsorbed during the 150 K dose. During the first TPD run, HCl desorption is observed, and there probably is also H₂ desorption above 300

K, although our mass spectrometer background at mass 2 is too large to allow direct observation of the relatively small signal for H₂ desorption from a coverage of clusters.

During the 2nd and subsequent TPD runs, substantial signals are observed for C₂D₄ desorption, indicating that HCl (and H₂) desorption during the 1st run exposed Pt sites. There is a low-temperature feature with about 1/3rd the intensity of that seen for Al₂O₃, which we attribute to C₂D₄ desorbing from alumina defect sites that were unblocked during the 1st TPD. The high temperature feature has about 46% the intensity of the high temperature feature observed for Pt₇/Al₂O₃ in the 1st TPD, suggesting that a significant fraction of the exposed Pt binding sites are still blocked, presumably by Sn. Critically, however, little if any D₂ desorption is observed. Note also that the ethylene desorption is essentially unchanged in four additional TPD runs.

The bottom frame of the figure shows the results of depositing Pt₇ on pre-heated, Sn-modified Al₂O₃. As noted above, this results in the deposition of 16.4 Sn atoms/10 nm² – about 2/3rd the amount present when Sn deposition is done after Pt₇ deposition. The C₂D₄ TPD results are actually quite similar to those observed when Sn is deposited after the clusters, with the exception that significant C₂D₄ desorption is observed in the 1st TPD. That simply reflects the fact that the heat/FT/Al₂O₃ sample was heated to desorb H and Cl prior to Pt₇ deposition, so that binding sites on both the alumina support and the clusters were available to binding C₂D₄. Again, little D₂ desorption is observed, and the high-temperature C₂D₄ desorption is reasonably stable in repeated TPD runs.

There are several interesting points. Little D₂ is observed even in the 1st TPD run, indicating that the Pt₇ cluster dehydrogenation properties were already strongly modified by the Sn, even though there was not Sn deposited directly onto the clusters. This suggests that some Sn may have diffused to the clusters, even though most of the clusters were deposited at cryogenic temperatures, and

were never heated prior to the TPD run. It is also possible that the clusters deposited on or immediately adjacent to Sn on the surface, and obtained some Sn modification in this way. It can also be seen that there is a significant change in the C₂D₄ desorption between the 1st and 2nd TPD runs, with the amount desorbing between ~200 and 300 K dropping significantly. This suggests that during the heating accompanying the 1st TPD run, the clusters changed somehow, and either additional Sn diffused to the clusters, in addition, the cluster morphology is likely to have evolved during the TPD heating. ISS experiments to probe changes in morphology are discussed next.

It is interesting to compare the behavior shown here for sub-nano PtSn clusters/alumina to that seen for sub-nano borated Pt_nB_m clusters/alumina,³⁵ and for ordered PtSn surface alloys.^{27, 28} In all three cases, ethylene dehydrogenation is strongly suppressed, compared to pure Pt_n/alumina or Pt(111), however, there are several important differences. In the case of PtSn surface alloys, the ethylene desorption temperature dropped with increasing Sn coverage from ~285 K for pure Pt(111)⁵⁸ to 184 K for the $\sqrt{3}\times\sqrt{3}$ R30° alloy. That alloy has a 1:2 Sn:Pt ratio in the surface layer, i.e., significantly lower than the Sn:Pt ratio in our clusters. For pure Pt clusters on alumina, the ethylene desorption occurs in a broad feature peaking near 300 K (Fig. 2a), and after boration, the desorption temperature drops substantially, peaking at cryogenic temperatures (overlapping the desorption from the alumina support). Thus, for both the extended PtSn alloy surfaces and Pt_nB_m/alumina, a substantial reduction in ethylene binding energy is at least partly responsible for the suppression of dehydrogenation – the ethylene desorbs before the onset of dehydrogenation. From the perspective of catalyzing selective alkane-to-alkene dehydrogenation, the reduction in alkene binding energy may be problematic, because that implies that the exothermicity of the $\text{alkane}_{\text{adsorbed}} \rightarrow \text{alkene}_{\text{adsorbed}}$ reaction is lower, which would tend to increase the activation energy.

In contrast, for the Sn-doped Pt₇/alumina clusters, the ethylene desorption feature remained above room temperature, with peak desorption temperature actually *increasing* relative to that for Sn-free Pt clusters. Nonetheless, dehydrogenation and the accompanying carbon deposition are suppressed, indicating that there must be another mechanism operating. A similar effect was predicted for supported PtGe, so far purely from theory.⁵⁹

Another interesting difference is that in the PtSn surface alloys the saturation ethylene coverage was unaffected by Sn surface concentration, but in both borated and Sn-alloyed Pt_n/alumina, the saturation coverages decreased significantly, by on the order of 50% in both cases. This difference may simply reflect a lower Sn:Pt ratio in the surface layer of the extended alloys (Sn:Pt \leq 1:2) compared to the levels of boron (\sim 1:1 B:Pt) and tin in the cluster experiments. As noted, the additional Sn deposited when Pt₇ was present corresponded to only 4 Sn/Pt₇, but the experiments where Pt₇ was deposited after Sn-treating the alumina support suggest that Sn initially on the alumina support diffuses to the clusters, raising the Sn:Pt ratio. Campbell reviewed chemisorption of small molecules on numerous bimetallic surface alloys and overlayer systems,⁶⁰ and also discussed the weaker binding of small molecules (NO and CO) on the exothermic PtSn alloy that resulted in significant decrease (>100 K) of desorption temperatures.⁶¹ For ethylene adsorption, a variety of different effects have been observed, ranging from simple site blocking to strong electronic effects on binding energies. In our clusters, Sn (and B) reduce the saturation ethylene coverage, presumably due to blocking of Pt sites. In addition, however, boration reduces the negative charge on the Pt clusters. Electronic effects of Sn addition are discussed below in the context of our DFT results.

The other important point from a catalysis perspective is that the high-temperature C₂D₄ desorption feature for the Sn-treated clusters was essentially unchanged in six TPD runs, whereas the

analogous feature for Pt₇/alumina decreased rapidly. This enhanced stability in repeated TPD cycling is not unexpected, since there is substantial carbon deposition for pure Pt_n/alumina model catalysts under these conditions,³³ however, it also indicates that the Sn-treated clusters must be reasonably stable with respect to sintering. This conclusion is consistent with calorimetric experiments by Anres *et al.* which found that bulk PtSn has a highly negative enthalpy of formation,⁶² which would slow the sintering kinetics in Campbell's modeling of sintering kinetics.^{63, 64} Similarly, Liu and Ascencio reported DFT and MD simulations for clusters of a few hundred atoms, finding that PtSn clusters were more energetically favorable than pure Pt clusters⁶⁵ Results of our DFT calculations for sub-nano PtSn clusters are presented below.

Low energy He⁺ scattering (ISS)

Example raw ISS spectra for select samples are shown in Fig. S1. More than 99% of He⁺ impinging on surfaces either neutralizes or implants in the surface, and thus the ISS signal corresponds to the small fraction of He⁺ ions that survive and backscatter along the surface normal.⁶⁶ Peaks in ISS result primarily from events in which an He⁺ scatters from a single atom in the top-most layer of the surface. Scattering from atoms deeper in the sample, or scattering involving multiple surface atoms is weak due to a combination of shadowing, blocking, and reduced ion survival probability (ISP), contributing mainly to the weak background observed at low E/E₀. Thus, the intensities of ISS peaks are highly sensitive to sample structure, including

cluster geometry and the presence of adsorbed species on top of cluster atoms. In the following, we present ISS data in the form of ISS peak intensities as a function of exposure to the He^+ beam, which slowly sputters the surface, providing some depth information. The intensities are normalized to the total scattered intensity in order to correct for any day-to-day changes in the He^+ beam flux.

Fig. 3 compares ISS sputter series results for $\text{Pt}_7/\text{Al}_2\text{O}_3$, $\text{FT}/\text{Pt}_7/\text{Al}_2\text{O}_3$, and $\text{Pt}_7/\text{heat}/\text{FT}/\text{Al}_2\text{O}_3$ samples. These measurements were done on a separate set of samples, but are directly comparable to the XPS and TPD data in Figs. 1 and 2. In each ISS experiment, the as-prepared sample was first exposed to two ISS scans at low ($0.2 \mu\text{A}$) He^+ flux. Then the sample was flashed to 700 K, driving the same

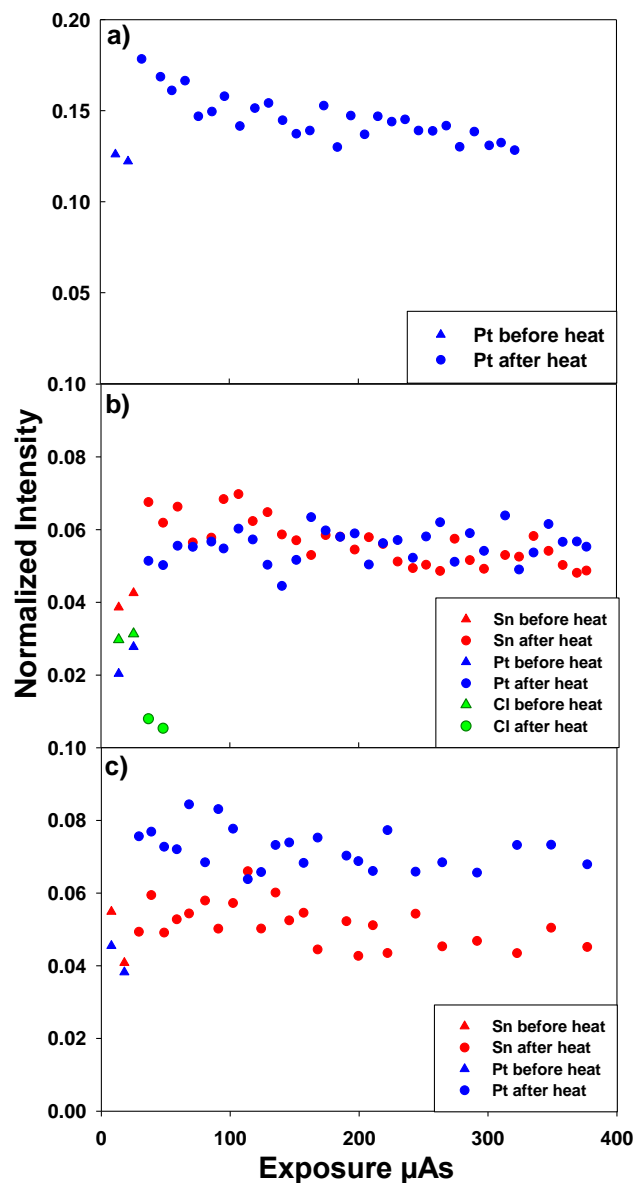


Figure 3. ISS intensities vs. He^+ exposure for: a) $\text{Pt}_7/\text{Al}_2\text{O}_3$, b) $\text{FT}/\text{Pt}_7/\text{Al}_2\text{O}_3$, c) $\text{Pt}_7/\text{heat}/\text{FT}/\text{Al}_2\text{O}_3$. In each experiment, 2 ISS scans were taken for the as-prepared sample, followed by a 700 K flash, and a series of ISS scans. “FT” refers to the full $\text{H}_2/\text{SnCl}_4/\text{H}_2$ treatment.

processes that would have occurred in other 700 K heating experiments, including TPD. Finally, repeated ISS scans were used to measure changes in the peak intensities as the sample was slowly sputtered.

The top frame shows the Pt ISS intensity for a Pt₇/Al₂O₃ sample. The first two points are for the as-deposited sample, and the rest are for the sample after flashing to 700 K. The increase in Pt intensity after flashing is attributed to desorption of adventitious adsorbates, primarily CO, which adsorbs very efficiently on samples with sub-nanometer dispersed clusters due to substrate-mediated adsorption (reverse spillover). Pt₇ desorption was done as the samples cooled from room temperature to ~120 K. This is above the temperature for CO desorption from the alumina support,⁶⁷ however, the lifetime of CO on the alumina is sufficient to allow some diffusion, thus allowing CO initially landing on the alumina to bind at a nearby Pt₇ cluster. After heating, the Pt ISS intensity slowly decreased, consistent with the slow sputtering of Pt from the surface.

For the as-prepared FT/Pt₇/Al₂O₃ sample, both Sn and Pt ISS peaks are observed, but with much lower intensity compared to the Pt peak intensity in the Pt₇/Al₂O₃ sample. This low intensity reflects the presence of Sn bound to the Pt cluster and of Cl and H atoms adsorbed on Pt and Sn sites, attenuating ISS from the underlying atoms by a combination of shadowing, blocking, and reduced ISP. The presence of Cl is confirmed by the appearance of a weak peak for Cl ISS, as shown in the figure. After heating, the Cl intensity is attenuated nearly to the background level, and the Pt and Sn intensity both increase. Because ISP varies significantly for different elements, it is not possible to infer the ratio of Sn/Pt in the surface layer from the Sn/Pt intensity ratio. Note, however, that just after heating, the Sn intensity is higher than that for Pt, but it decays with time, while the Pt intensity is nearly constant (unlike the slow decline observed for Pt₇/Al₂O₃). This behavior indicates that the sputter rate for Sn is faster than that for Pt, which could reflect differences in the binding energy to the surface, but also would be expected if the heated clusters have Sn in the surface layer.

For the Pt₇/heat/FT/Al₂O₃ sample (bottom frame), the initial Sn ISS intensity is similar to that for the FT/Pt₇/Al₂O₃ sample, but the Pt intensity is twice as high as Pt in that sample. This is expected. The number of Sn atoms on the surface of both samples is high, but for FT/Pt₇/Al₂O₃, the Pt₇ has Sn, Cl, and H adsorbed on top, while for Pt₇/heat/FT/Al₂O₃, the Pt clusters are deposited on top after desorbing H and Cl, and thus should have less adsorbate coverage. Interestingly, however, the initial Pt intensity for Pt₇/heat/FT/Al₂O₃ is still only ~40% of that for the Pt₇/Al₂O₃ sample. This implies that even though the Pt clusters were deposited after the substrate was Sn-modified and heated, something is attenuating ISS from the Pt atoms. The most likely possibility is that some Sn atoms have aggregated to the clusters, which, given the ~0.1 ML coverage of Sn in these samples, is not surprising. If the Sn is initially present as isolated atoms, the average Sn-Sn separation is less than 1 nm, and there would be a high probability for Pt₇ clusters to deposit on top of, or very near to Sn atoms on the substrate. Again, cluster isomerizing to flatter shapes that favor Pt-Sn binding cannot be ruled out. Both suppositions that Sn already is binding to the clusters as-deposited would also explain why no significant D₂ desorption is observed in the 1st TPD on the Pt₇/heat/FT/Al₂O₃ sample – the clusters are already Sn-modified.

After heating, the Sn intensity in the Pt₇/heat/FT/Al₂O₃ sample was essentially unchanged, but the Pt intensity increased by nearly a factor of two. Some of this increase can be attributed to the desorption of adventitious CO (as in the Pt₇/Al₂O₃ data in the top frame), but there may also be some restructuring of the clusters.

DFT Calculations

Because the Sn-modified Pt clusters are quite large, and the number of Sn atoms present is not well defined, it was not feasible to try to compute the structures. We previously reported on the structures of Pt₇/Al₂O₃ with and without 1-3 ethylene molecules adsorbed.³³ Here we report DFT

calculations of structures, atomic charges, and ethylene binding behavior for a small model system, consisting of Pt_4Sn_3 clusters on an alumina support.

The global optimization was carried out, with the purpose of finding the low-lying minima that could be thermally populated at temperatures of the TPD. The three lowest energy structures found for Pt_4Sn_3 /alumina are shown in

Fig. 4, with the atomic charges, energies relative to the global minimum structure, and the Boltzmann populations estimated at 700 K. The Pt_4Sn_3 clusters were all singlets with a net negative charge indicating net electron transfer from the alumina support to the clusters (see Table S4). The structures also tend to have Pt binding to underlying Al atoms, while the Sn binds to both Al and O atoms on the surface.

The global minimum structure is nearly planar with all atoms exposed in the surface layer. The Sn atoms are all positively

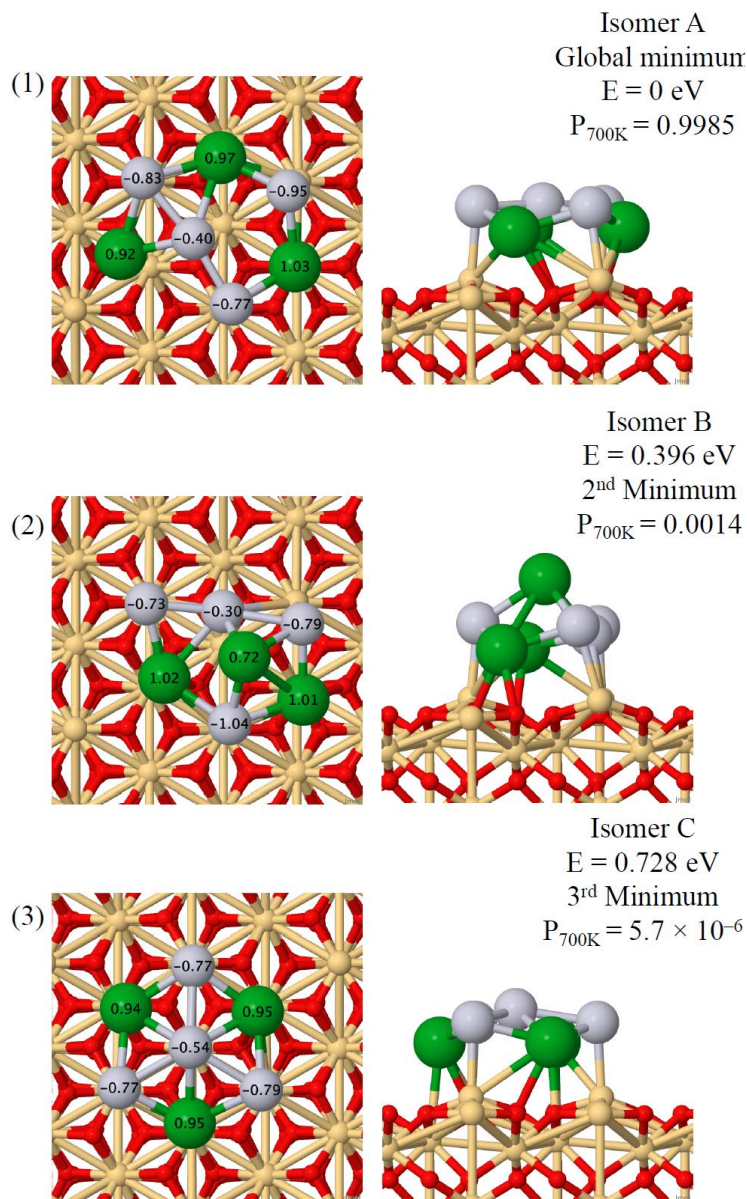


Figure 4. (1) Isomer A, the global minimum structure for Pt_4Sn_3 /alumina. (2) Isomer B, the 2nd minimum structure for Pt_4Sn_3 /alumina. (3) Isomer C, the 3rd minimum. E indicates the energy relative to the global minimum structure. $P_{700\text{K}}$ is the Boltzmann population at 700 K.

charged by nearly 1 e, and the Pt atoms are negative, with charges ranging from -0.4 e to -0.95 e, thus, there is substantial electron transfer from Sn to Pt. The charge distribution is consistent with the high Sn 3d BEs measured by XPS, which indicates oxidized Sn. The Sn and Pt atoms are mixed, rather than phase-separated.

The second minimum structure is substantially (0.396 eV) higher in energy than the global minimum, thus even at 700 K, its predicted population remains below 1 %. Again, the Sn atoms are all positively charged by $\sim 1e$, and the Pt atoms are negative, with charges between -0.3 and -1.04 e. This structure is three dimensional, with a Sn atom in the top layer. The third isomer is a roughly hexagonal, quasi-planar structure with alternative Pt and Sn atoms around the periphery, but it is >0.7 eV above the global minimum and has near-zero population at 700 K. Again, there is substantial Sn-to-Pt electron transfer. One important observation can be made about the global minimum that both Sn and Pt atoms are in contact with the support. This kind of structure could form either if Sn is deposited on alumina-supported Pt clusters and the cluster restructures upon heating, or if Sn is on the surface before the Pt cluster arrives and it mixes into Pt upon heating. Hence both of our aforementioned hypotheses of the effect of heating on the ethylene binding remain valid, and in fact they might be indistinguishable.

DFT calculations were also performed for ethylene binding to the three Pt_4Sn_3 /alumina structures. A total of 10 structures were found to be within thermal reach, as shown in Fig. 5. Again, the Sn atoms are positively charged by roughly 1 e each, and the Pt atoms are negatively charged by -0.4 e to -1 e. There are several interesting points. Note that the two lowest energy structures for

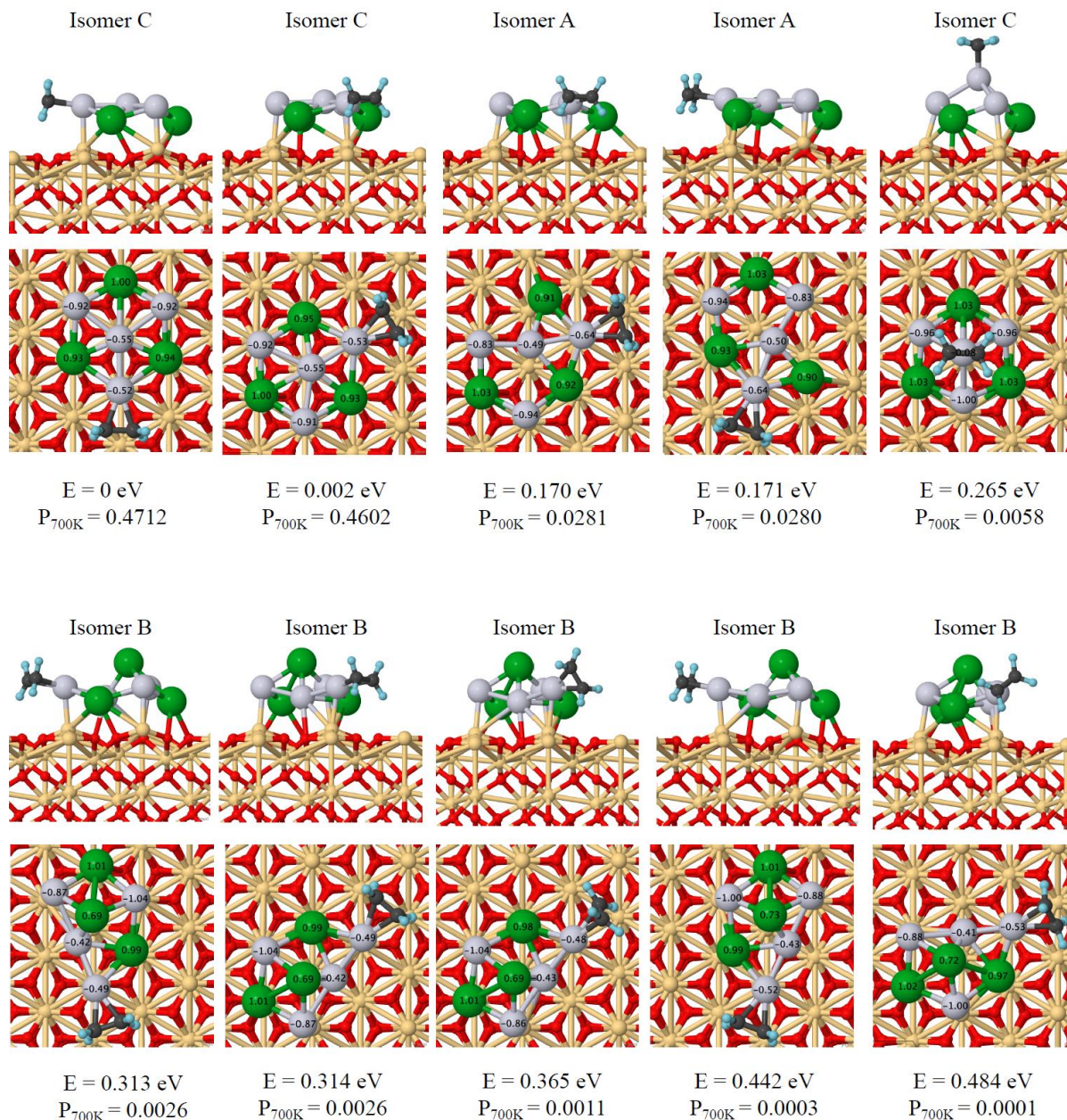


Figure 5. Structures of Pt_4Sn_3 /alumina with one ethylene bound, with energies relative to the global minimum (GM), and thermal populations at 700 K. Note that the GM with ethylene is based on Isomer C of the bare cluster.

C₂H₄/Pt₄Sn₃/alumina are based on ethylene binding to Isomer C of Pt₄Sn₃/alumina, which is ~0.4 eV above the global minimum for the bare cluster. These two nearly isoenergetic structures both have C₂H₄ π -bonded to a single Pt atom around the edge of the nearly planar Isomer C structure. The 3rd and 4th isomers are built on Isomer A, i.e., the global minimum for Pt₄Sn₃/alumina, and again are nearly isoenergetic structures with C₂H₄ π -bonded to single Pt atoms at the edge of the cluster. The 5th isomer is again built on Isomer C of Pt₄Sn₃/alumina, but in this case has C₂H₄ bound on top of the cluster, with substantial distortion of the cluster. This 5th isomer is already 0.265 eV above the global minimum, and thus has <1% population weighting at 700 K. The other 5 structures are all built on Isomer B of Pt₄Sn₃/alumina, and have energies between 0.313 and 0.444 eV above the global minimum, hence having very small population weighting.

It is interesting to compare these structures to those found for ethylene bound to Pt_n/alumina previously. For the Sn-free Pt clusters, ethylene binds in both π and di- σ geometries (i.e., with each C atom bound to a different Pt atom, and sp² hybridization broken). Di- σ bonding has been associated with a propensity for dehydrogenation, thus the DFT structures are consistent with the observation of significant D₂ desorption from the Sn-free Pt₇/alumina sample. In contrast, all the structures found for Pt₄Sn₃/alumina have only π -bonding of ethylene, which is presumably a factor contributing to the observation that little D₂ is generated for Sn-treated Pt₄Sn₃/alumina. We confirmed the strong correlation between the mode of binding of ethylene and the barrier to dehydrogenation for other co-alloying elements, Si and Ge^{59, 68}. The barriers associated with ethylene undergoing dehydrogenation from the π -mode is typically several times larger than that for the di- σ mode. In addition, upon dehydrogenation, a detached H atom needs to bind to Pt, and, when most of Pt atoms are separated by Sn, the sites for H atom arrival becomes unavailable. In contrast, for the preceding step of ethane dehydrogenation, there is no need for two adjacent Pt

sites, as the reaction occurs on a single Pt atom⁵⁹. Hence, in agreement with the experiment, theory shows that PtSn clusters should prevent dehydrogenation of alkanes beyond olefins.

CONCLUSIONS

We have shown that an ALD-like process can be used to modify Pt₇/alumina samples with Sn, both before and after Pt cluster deposition. Sn deposition is roughly 5 to 6 times more efficient on Pt sites than on the alumina support; however, it is far less selective for Pt sites than the Pt_n/SiO₂, studied previously. Modification of the alumina (e.g. use of thicker, less defective thin films) would presumably reduce the number of alumina sites that support Sn deposition, making the process more selective for Pt sites.

For these model catalysts, Sn modification almost completely suppresses carbon deposition, i.e. coking, and unlike the B-induced suppression of coking, it does it without lowering the ethylene binding energy. The effects of adding Sn to the support before depositing clusters, vs. depositing Sn after cluster deposition, are quite similar, and both the TPD and ISS results indicating that Sn present on the support prior to Pt₇ deposition must be binding to, and modifying the chemical properties of the Pt clusters, even at the low deposition temperatures.

The DFT results show that Sn and Pt mix intimately, with substantial Pt-to-Sn electron transfer. The clusters have exclusively spin-singlet isomers, and ethylene binds to Pt in PtSn in an exclusively π -mode. In contrast, Sn-free Pt clusters have both closed and open-shell structures, allowing ethylene to bind strongly in di- σ geometries that tend to undergo dehydrogenation, rather than desorption. The electronic, structural, and mechanistic effects of Sn closely resemble those for Si and Ge recently predicted theoretically.

Sn-modification clearly makes two highly desirable changes to sub-nano Pt_n/alumina catalysts for potential applications in fuel-rich, high-temperature applications. First, it almost completely suppresses dehydrogenation to deposit carbon on the surface. In addition, repeated TPD experiments show very little run-to-run change in the C₂D₄ desorption intensity or temperature dependence, indicating that the catalysts are also more thermally stable than Sn-free Pt_n clusters on alumina. Both factors would be highly desirable in applications where the catalysts must be stable against coking and sintering. One such application is alkane-to-alkene dehydrogenation as an endothermic reaction for air vehicle cooling. The gas-phase Sn deposition process used could, presumably, be adapted to modifying small Pt clusters supported on alumina-coated lines and other fuel system parts.

SUPPLEMENTARY MATERIAL

Details of the XPS intensity correction process, example raw ISS spectra, and coordinates of the DFT structures can be found in the supplementary information.

Acknowledgments

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Supporting Information

Table S1. XPS data calibration: The thickness of the alumina film was different for different samples, so the total number of electrons passing out of the film were at different values. We can assume that the thickness was all same at 4.7 nm, by calculating the number of electrons passing out of all the different films, then find the relative percentage decrease that is required for the Al intensities of original XPS data thicker films and that brings us the values for “Al peak intensities after correction to same thickness”. We then assume that all these Al intensities should be of the same value as that of the Pt₇-Al₂O₃ sample and hence all the obtained XPS data were scaled up by percentages listed in the last column of table S1.

	Al ₂ O ₃ thickness (nm)	Al 2s peak intensities of original XPS data	Al 2s peak intensity after correction to same thickness	Percentage increased for XPS data normalization
Pt ₇ /Al ₂ O ₃	5.3	56605	54972	0%
FT/Al ₂ O ₃	5.2	43209	42141	30%
Heat/FT/Al ₂ O ₃	5.2	45678	44549	23%
FT/Pt ₇ /Al ₂ O ₃	5.7	47755	45688	20%
Heat/FT/Pt ₇ /Al ₂ O ₃	5.7	54398	52043	6%
Pt ₇ /heat/FT/Al ₂ O ₃	4.7	33667	33667	63%
Heat/Pt ₇ /heat/FT/Al ₂ O ₃	4.7	32246	32246	70%
Pt ₇ /heat/FT/Al ₂ O ₃ post 6 TPDs	4.7	46671	46671	18%

Table S2. Binding energies of Pt 4d 5/2 and Sn 3d 5/2 peaks taken from figure 1. Results were calibrated by using the binding energy, from O 1s in Al₂O₃, of 531.7 eV.

Binding energy in XPS	Pt 4d 5/2	Sn 3d 5/2
Pt ₇ /Al ₂ O ₃	315.4 eV	
FT/Al ₂ O ₃		487.9 eV
Heat/FT/Al ₂ O ₃		487.6 eV
FT/Pt ₇ /Al ₂ O ₃	316.2 eV	487.9 eV
Heat/FT/Pt ₇ /Al ₂ O ₃	315.5 eV	487.1 eV
Pt ₇ /heat/FT/Al ₂ O ₃	315.7 eV	487.3 eV
Heat/Pt ₇ /heat/FT/Al ₂ O ₃	315.5 eV	487.1 eV

Table S3 Molecules desorbed per cluster for C₂D₄ and D₂ from experimental samples quantified from figure 2, assuming all molecules desorbed were from the clusters. C₂D₄ and D₂ molecules desorbed were quantified by taking the integral of the desorption peaks (range was 130 K to 500 K), then were divided by the number of Pt clusters in the area of analysis. Corresponding to 0.1 ML of Pt coverage and 0.0314 cm² of cluster spot size on the sample, 6.73×10^{11} of clusters in the area of analysis were assumed for the TPD calculations.

	1 st TPD	2 nd TPD	3 rd TPD	4 th TPD	5 th TPD	6 th TPD
Pt ₇ /Al ₂ O ₃	8.64 5.44 4.30 1.44					
C ₂ D ₄						
D ₂						
FT/Pt ₇ /Al ₂ O ₃	0.70 4.52 4.43 4.32 4.12 3.88 0.03 0.13 0.15 0.15 0.06 0.10					
C ₂ D ₄						
D ₂						
Pt ₇ /heat/FT/Al ₂ O ₃	4.53 4.28 4.19 4.33 3.58 3.67 0.55 0.40 0.24 0.35 0.10 0.21					
C ₂ D ₄						
D ₂						
Blank Al ₂ O ₃	1.63					
C ₂ D ₄						

Molecules desorbed conversion

We start by leaking in 2×10^{-8} Torr of ethylene into the main chamber and the electronics recorded the corresponding number of counts per second.

We then correct for the pressure from the 2×10^{-8} Torr of ethylene that was leaked in,

$$\text{Corrected pressure} = 2 \times 10^{-8} \text{ Torr} \times \text{ion gauge sensitivity factor} \quad (1)$$

Then calculate the molecular density from the corrected pressure by:

$$\rho = \text{corrected pressure} \times N_A/RT \quad (2)$$

We now calculate velocity of the gas molecule,

$$V_{rms} = 158\sqrt{T/m(\text{atomic wt of molecule})} \quad (3)$$

And the flux of molecules into the mass spectrometer,

$$Z_{wall} = 0.25 \times \rho \times V_{rms} \quad (4)$$

Which leads to molecules entering the mass spectrometer per second,

$$\text{molecules entering mass spec per second} = Z_{wall} \times \text{aperture area of the skimmer cone on the mass spec} \quad (5)$$

Finally, we obtain molecules per count from molecules entering mass spec per second divided by the number of counts per second as recorded in electronics from leaking in ethylene in the first step of this conversion,

$$\text{Molecules per count} = \frac{\text{molecules entering mass spec/second}}{\text{number of counts/second}} \quad (6)$$

The calibration is not yet finished as in any raw TPD data, a total of 8 different masses were observed, the first mass is scanned for 0.05 seconds followed by a wait time then another mass is scanned, this is repeated for all 8 masses, therefore it takes around 1.2 seconds for the electronics to return to scanning the first mass again. This cycle is defined as a duty cycle and the count time of 0.05 seconds divided by the duty cycle is defined as the duty factor.

The TPD results collected were initially in counts, this is divided by the duty factor to obtain the true counts, then multiplied by the molecules per count obtained in (6) to produce the final results in figure 2.

Figure S1. Raw ISS spectrum of Heat/Pt₇/Al₂O₃ (blue) and Heat/FT/Pt₇/Al₂O₃ (red). O, Al, Sn and Pt peaks are labeled. Cl is labeled around the area where it would exist if present on surface of the samples.

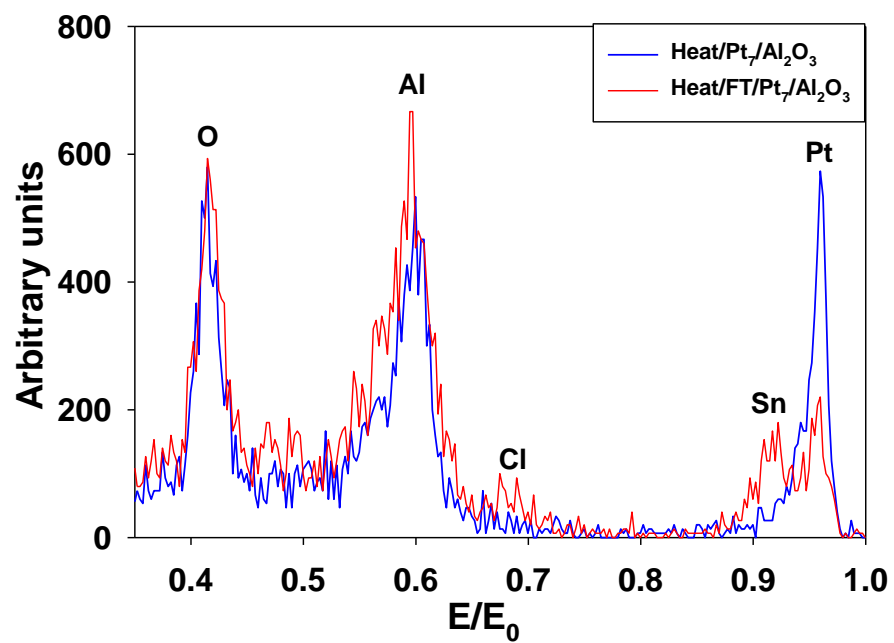


Table S4. DFT calculations for Pt₄Sn₃ on alumina. E is the energy relative to global minimum, 2S+1 is the spin multiplicity and Q_{cluster} is the net charge of the cluster.

Isomer	E(eV)	2S+1	Q_{cluster}(e)
A	0	1	-0.04
B	0.396	1	-0.1
C	0.728	1	-0.03
D	0.756	1	-0.07

Table S5 DFT calculations for ethylene binding Pt_4Sn_3 on alumina. E is the energy relative to global minimum, $2S+1$ is the spin multiplicity and Q_{cluster} is the net charge of the cluster. Mode means the type of interaction between ethylene and cluster. C-C is the distance between the two carbon on ethylene.

Isomer	E(eV)	$2S+1$	$Q_{\text{cluster}}(\text{e})$	Mode	C-C(A)
C	0	1	-0.03	pi	1.41
C	0.001	1	-0.03	pi	1.41
A	0.170	1	-0.04	pi	1.40
A	0.171	1	-0.04	pi	1.40
C	0.265	1	0.08	pi	1.43
B	0.313	1	-0.13	pi	1.41
B	0.314	1	-0.12	pi	1.41
B	0.365	1	-0.12	pi	1.41

Figure 4

Coordinates for Pt₄Sn₃, the format is

Number of atom

Comment line: cluster-support-isomer

symbol x y z bader_charge

277				
pt4sn3-al2o3-A				
Al	9.69003000	2.79452000	0.00000000	2.16903200
Al	4.84978000	11.17808000	0.00000000	2.16893610
Al	0.00953000	2.79452000	0.00000000	2.16899470
Al	7.26991000	6.98630000	0.00000000	2.16889230
Al	-4.83072000	11.17808000	0.00000000	2.16890010
Al	-2.41059000	6.98630000	0.00000000	2.16899870
Al	4.84978000	2.79452000	0.00000000	2.16886050
Al	0.00953000	11.17808000	0.00000000	2.16895800
Al	2.42966000	6.98630000	0.00000000	2.16901000
O	10.62741000	1.39726000	0.85241000	-1.55246510
O	12.85153000	0.11316000	0.85241000	-1.56066860
O	12.85153000	2.68136000	0.85241000	-1.55848090
O	5.78716000	9.78082000	0.85241000	-1.55217950
O	8.01128000	8.49672000	0.85241000	-1.56064900
O	8.01128000	11.06492000	0.85241000	-1.55830160
O	0.94691000	1.39726000	0.85241000	-1.55238230
O	8.20728000	5.58904000	0.85241000	-1.55242460
O	10.43141000	4.30494000	0.85241000	-1.56100600
O	3.17103000	0.11317000	0.85241000	-1.56066520
O	10.43140000	6.87314000	0.85241000	-1.55839870
O	3.17103000	2.68136000	0.85241000	-1.55831920
O	-3.89334000	9.78082000	0.85241000	-1.55245030
O	-1.66922000	8.49672000	0.85241000	-1.56080070
O	-1.66922000	11.06492000	0.85241000	-1.55842250
O	-1.47322000	5.58904000	0.85241000	-1.55253340
O	5.78716000	1.39726000	0.85241000	-1.55228330
O	8.01128000	0.11317000	0.85241000	-1.56068690
O	0.75091000	4.30494000	0.85241000	-1.56061740
O	0.75090000	6.87314000	0.85241000	-1.55846130
O	8.01128000	2.68136000	0.85241000	-1.55840140
O	0.94691000	9.78082000	0.85241000	-1.55240040
O	3.17103000	8.49672000	0.85241000	-1.56048260
O	3.17103000	11.06492000	0.85241000	-1.55834490

O	3.36703000	5.58904000	0.85241000	-1.55220470
O	5.59116000	4.30494000	0.85241000	-1.56062530
O	5.59116000	6.87314000	0.85241000	-1.55825850
Al	2.42965000	12.57534000	1.70482000	2.46326480
Al	4.84978000	8.38356000	1.70482000	2.46327080
Al	-7.25084000	12.57534000	1.70482000	2.46327130
Al	7.26991000	4.19178000	1.70482000	2.46335990
Al	-4.83072000	8.38356000	1.70482000	2.46337230
Al	-2.41059000	4.19178000	1.70482000	2.46349420
Al	-2.41060000	12.57534000	1.70482000	2.46340340
Al	0.00953000	8.38356000	1.70482000	2.46336390
Al	2.42966000	4.19178000	1.70482000	2.46323490
Al	12.11016000	1.39726000	2.20274000	2.48269380
Al	7.26991000	9.78082000	2.20274000	2.48268280
Al	9.69003000	5.58904000	2.20274000	2.48279730
Al	2.42966000	1.39726000	2.20274000	2.48277460
Al	-2.41059000	9.78082000	2.20274000	2.48282750
Al	7.26991000	1.39726000	2.20274000	2.48275630
Al	0.00953000	5.58904000	2.20274000	2.48269450
Al	2.42966000	9.78082000	2.20274000	2.48280940
Al	4.84978000	5.58904000	2.20274000	2.48271940
O	8.94865000	1.28410000	3.05515000	-1.64220590
O	11.17279000	0.00001000	3.05515000	-1.62408920
O	4.10840000	9.66766000	3.05515000	-1.64211630
O	11.36879000	2.90768000	3.05515000	-1.64999060
O	6.33254000	8.38356000	3.05515000	-1.62409530
O	6.52853000	5.47588000	3.05515000	-1.64192820
O	-0.73185000	1.28410000	3.05515000	-1.64217340
O	6.52853000	11.29124000	3.05515000	-1.64987110
O	1.49229000	0.00001000	3.05515000	-1.62406150
O	8.75266000	4.19179000	3.05515000	-1.62430730
O	-5.57210000	9.66766000	3.05515000	-1.64198580
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O	1.68828000	2.90768000	3.05515000	-1.65005510
O	-3.34797000	8.38357000	3.05515000	-1.62431670
O	4.10840000	1.28410000	3.05515000	-1.64198310
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O	-0.92784000	4.19178000	3.05515000	-1.62435330
O	6.33254000	0.00001000	3.05515000	-1.62426730
O	6.52854000	2.90768000	3.05515000	-1.64989760
O	-0.73185000	9.66766000	3.05515000	-1.64219040
O	-0.73184000	7.09946000	3.05515000	-1.65024200

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O	1.68829000	11.29124000	3.05515000	-1.64999700
O	1.68828000	5.47588000	3.05515000	-1.64215390
O	3.91241000	4.19178000	3.05515000	-1.62409670
O	4.10841000	7.09946000	3.05515000	-1.64980420
Al	9.69003000	2.79452000	3.90756000	2.47804340
Al	4.84978000	11.17808000	3.90756000	2.47790610
Al	0.00953000	2.79452000	3.90756000	2.47792840
Al	7.26991000	6.98630000	3.90756000	2.47778690
Al	-4.83072000	11.17808000	3.90756000	2.47782460
Al	-2.41059000	6.98630000	3.90756000	2.47804610
Al	4.84978000	2.79452000	3.90756000	2.47779910
Al	0.00953000	11.17808000	3.90756000	2.47788640
Al	2.42966000	6.98630000	3.90756000	2.47799910
Al	2.42965000	12.57534000	4.40548000	2.47224150
Al	4.84978000	8.38356000	4.40548000	2.47240090
Al	-7.25084000	12.57534000	4.40548000	2.47235490
Al	7.26991000	4.19178000	4.40548000	2.47221690
Al	-4.83072000	8.38356000	4.40548000	2.47227490
Al	-2.41059000	4.19178000	4.40548000	2.47227870
Al	-2.41060000	12.57534000	4.40548000	2.47230300
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Al	2.42966000	4.19178000	4.40548000	2.47247260
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O	3.36702000	11.17808000	5.25789000	-1.64355920
O	5.59116000	12.46219000	5.25789000	-1.65405600
O	5.59116000	9.89398000	5.25789000	-1.64903520
O	-1.47322000	2.79452000	5.25789000	-1.64355830
O	5.78715000	6.98630000	5.25789000	-1.64320310
O	8.01128000	8.27041000	5.25789000	-1.65410360
O	0.75091000	4.07863000	5.25789000	-1.65393910
O	0.75091000	1.51042000	5.25789000	-1.64897050
O	8.01129000	5.70220000	5.25789000	-1.64905180
O	-6.31347000	11.17808000	5.25789000	-1.64334670
O	-4.08934000	12.46219000	5.25789000	-1.65405740
O	-4.08934000	9.89398000	5.25789000	-1.64918400
O	-3.89335000	6.98630000	5.25789000	-1.64344260
O	3.36703000	2.79452000	5.25789000	-1.64357320
O	5.59116000	4.07863000	5.25789000	-1.65403930
O	-1.66922000	8.27041000	5.25789000	-1.65378550
O	5.59116000	1.51042000	5.25789000	-1.64908870

O	-1.66921000	5.70220000	5.25789000	-1.64910600
O	-1.47323000	11.17808000	5.25789000	-1.64348960
O	0.75091000	12.46219000	5.25789000	-1.65395160
O	0.75091000	9.89398000	5.25789000	-1.64895080
O	0.94690000	6.98630000	5.25789000	-1.64362280
O	3.17103000	8.27041000	5.25789000	-1.65379320
O	3.17104000	5.70220000	5.25789000	-1.64897440
Al	12.11016000	1.39726000	6.11030000	2.47609940
Al	7.26991000	9.78082000	6.11030000	2.47618780
Al	9.69003000	5.58904000	6.11030000	2.47609450
Al	2.42966000	1.39726000	6.11030000	2.47616750
Al	-2.41059000	9.78082000	6.11030000	2.47602880
Al	7.26991000	1.39726000	6.11030000	2.47600380
Al	0.00953000	5.58904000	6.11030000	2.47582370
Al	2.42966000	9.78082000	6.11030000	2.47611450
Al	4.84978000	5.58904000	6.11030000	2.47622030
Al	9.69003000	2.79452000	6.60910000	2.47675900
Al	4.84978000	11.17808000	6.60910000	2.47694100
Al	0.00953000	2.79452000	6.60910000	2.47670790
Al	7.26991000	6.98630000	6.60910000	2.47693160
Al	-4.83072000	11.17808000	6.60910000	2.47684900
Al	-2.41059000	6.98630000	6.60910000	2.47697910
Al	4.84978000	2.79452000	6.60910000	2.47663380
Al	0.00953000	11.17808000	6.60910000	2.47664420
Al	2.42966000	6.98630000	6.60910000	2.47695180
O	11.36395000	0.11351000	7.46570000	-1.64888900
O	11.37150000	2.68537000	7.46570000	-1.65015580
O	13.59502000	1.39291000	7.46570000	-1.65377190
O	6.52370000	8.49707000	7.46570000	-1.64827560
O	6.53125000	11.06893000	7.46570000	-1.64957150
O	8.75477000	9.77647000	7.46570000	-1.65366090
O	1.68345000	0.11351000	7.46570000	-1.64882940
O	8.94383000	4.30529000	7.46570000	-1.64966560
O	8.95137000	6.87715000	7.46570000	-1.64964460
O	1.69100000	2.68537000	7.46570000	-1.65026870
O	11.17490000	5.58469000	7.46570000	-1.65479370
O	3.91452000	1.39291000	7.46570000	-1.65384470
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O	-3.14925000	11.06893000	7.46570000	-1.64938120
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O	6.52370000	0.11351000	7.46570000	-1.64905820
O	-0.72913000	6.87715000	7.46570000	-1.65006750

O	6.53125000	2.68537000	7.46570000	-1.64926540
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O	1.68345000	8.49707000	7.46570000	-1.64900620
O	1.69100000	11.06893000	7.46570000	-1.64917780
O	3.91452000	9.77646000	7.46570000	-1.65380000
O	4.10358000	4.30529000	7.46570000	-1.64896320
O	4.11112000	6.87715000	7.46570000	-1.64892060
O	6.33465000	5.58469000	7.46570000	-1.65389130
Al	2.42965000	12.57534000	8.32833000	2.47127630
Al	4.84978000	8.38356000	8.32833000	2.47059540
Al	-7.25084000	12.57534000	8.32833000	2.47118140
Al	7.26991000	4.19178000	8.32833000	2.47181180
Al	-4.83072000	8.38356000	8.32833000	2.47227660
Al	-2.41059000	4.19178000	8.32833000	2.47178100
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Al	0.00953000	8.38356000	8.32833000	2.47087930
Al	2.42966000	4.19178000	8.32833000	2.47056480
Al	12.11016000	1.39726000	8.78548000	2.47180270
Al	7.26991000	9.78082000	8.78548000	2.47711810
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Al	-2.41059000	9.78082000	8.78548000	2.47201400
Al	7.26991000	1.39726000	8.78548000	2.47212220
Al	0.00953000	5.58904000	8.78548000	2.47259920
Al	2.42966000	9.78082000	8.78548000	2.47541800
Al	4.84978000	5.58904000	8.78548000	2.47643050
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O	10.45104000	1.30159000	9.68989000	-1.65748230
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O	8.18232000	8.39182000	9.68989000	-1.65696500
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Al	2.42966000	6.98630000	10.71830000	2.47968600
Al	2.42965000	12.57534000	10.98601000	2.47027630
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Al	-4.83072000	11.17808000	3.90756000	2.47777610
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O	5.78715000	6.98630000	5.25789000	-1.64296020
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Al	4.84978000	2.79452000	6.60910000	2.47681250
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O	13.59502000	1.39291000	7.46570000	-1.65387700
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O	-0.73667000	4.30528000	7.46570000	-1.64969740
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O	-0.72913000	6.87715000	7.46570000	-1.65002200
O	6.53125000	2.68537000	7.46570000	-1.64990120
O	8.75477000	1.39291000	7.46570000	-1.65384050
O	1.49440000	5.58468000	7.46570000	-1.65395130
O	1.68345000	8.49707000	7.46570000	-1.64937990
O	1.69100000	11.06893000	7.46570000	-1.64910540
O	3.91452000	9.77646000	7.46570000	-1.65382710
O	4.10358000	4.30529000	7.46570000	-1.64899030
O	4.11112000	6.87715000	7.46570000	-1.64892700
O	6.33465000	5.58469000	7.46570000	-1.65386240
Al	9.69003000	0.00000000	8.32833000	2.47028690
Al	4.84978000	8.38356000	8.32833000	2.47058470
Al	0.00954000	0.00000000	8.32833000	2.47048230
Al	7.26991000	4.19178000	8.32833000	2.47146440
Al	-4.83072000	8.38356000	8.32833000	2.47221030
Al	-2.41059000	4.19178000	8.32833000	2.47086540
Al	4.84978000	0.00000000	8.32833000	2.47152180
Al	0.00953000	8.38356000	8.32833000	2.47079530
Al	2.42966000	4.19178000	8.32833000	2.47119190
Al	12.11016000	1.39726000	8.78548000	2.47241810
Al	7.26991000	9.78082000	8.78548000	2.47612140
Al	9.69003000	5.58904000	8.78548000	2.46989550
Al	2.42966000	1.39726000	8.78548000	2.47283660

Al	-2.41059000	9.78082000	8.78548000	2.47257870
Al	7.26991000	1.39726000	8.78548000	2.47206760
Al	0.00953000	5.58904000	8.78548000	2.47177860
Al	2.42966000	9.78082000	8.78548000	2.47657780
Al	4.84978000	5.58904000	8.78548000	2.47587930
O	8.01661000	2.88194000	9.68989000	-1.64548650
O	3.17636000	11.26550000	9.68989000	-1.63946240
O	10.45104000	1.30159000	9.68989000	-1.65664550
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O	8.18232000	8.39182000	9.68989000	-1.65580500
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O	10.60245000	4.20004000	9.68989000	-1.66803450
O	3.34207000	0.00826000	9.68989000	-1.66708200
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O	0.77054000	9.68514000	9.68989000	-1.64486630
O	0.92195000	4.20004000	9.68989000	-1.66813610
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Al	9.69003000	2.79452000	10.71830000	2.47483110
Al	4.84978000	11.17808000	10.71830000	2.48232030
Al	0.00953000	2.79452000	10.71830000	2.47525980
Al	7.26991000	6.98630000	10.71830000	2.47214740
Al	-4.83072000	11.17808000	10.71830000	2.48123320
Al	-2.41059000	6.98630000	10.71830000	2.47551170
Al	4.84978000	2.79452000	10.71830000	2.47662770
Al	0.00953000	11.17808000	10.71830000	2.48035180
Al	2.42966000	6.98630000	10.71830000	2.47411790
Al	9.69003000	0.00000000	10.98601000	2.47086950
Al	4.84978000	8.38356000	10.98601000	2.47166380

Al	0.00954000	0.00000000	10.98601000	2.47435270
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Al	-4.83072000	8.38356000	10.98601000	2.46845230
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O	6.47008000	8.24776000	11.85616000	-1.59509680
O	-0.70378000	1.44405000	11.85056000	-1.62358840
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O	8.80259000	7.00237000	11.86964000	-1.61550810
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O	-3.23765000	8.27110000	11.85222000	-1.62160400
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O	6.38936000	2.86370000	11.86401000	-1.62146910
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O	1.65082000	8.29511000	11.86254000	-1.59271560
O	1.71573000	5.64161000	11.88061000	-1.62891850
O	3.95878000	7.02253000	11.94148000	-1.56805090
Al	12.10920000	1.39569000	11.90056000	2.41691370
Al	7.23784000	9.77592000	12.33353000	2.38327320
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Al	2.42883000	1.40120000	11.89288000	2.41593570
Al	-2.41630000	9.77630000	11.88779000	2.41470630
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Al	-0.00178000	5.58539000	11.84950000	2.41540230
Al	2.40441000	9.84991000	12.35186000	2.38379500
Al	4.85768000	5.53714000	12.39424000	2.37564080

Pt	2.32997000	9.72856000	14.77189000	-0.72846700
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Al	7.26991000	6.98630000	0.00000000	2.16904850
Al	-4.83072000	11.17808000	0.00000000	2.16910640
Al	-2.41059000	6.98630000	0.00000000	2.16903440
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Al	0.00953000	11.17808000	0.00000000	2.16902820
Al	2.42966000	6.98630000	0.00000000	2.16906510
O	10.62741000	1.39726000	0.85241000	-1.55200900
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O	3.17103000	8.49672000	0.85241000	-1.56033700
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O	5.59116000	4.30494000	0.85241000	-1.56029510
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Al	4.84978000	8.38356000	1.70482000	2.46327450
Al	0.00954000	0.00000000	1.70482000	2.46327530
Al	7.26991000	4.19178000	1.70482000	2.46324150
Al	-4.83072000	8.38356000	1.70482000	2.46320220
Al	-2.41059000	4.19178000	1.70482000	2.46324170
Al	4.84978000	0.00000000	1.70482000	2.46320300
Al	0.00953000	8.38356000	1.70482000	2.46324250
Al	2.42966000	4.19178000	1.70482000	2.46321220
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Al	7.26991000	9.78082000	2.20274000	2.48264390
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Al	2.42966000	1.39726000	2.20274000	2.48267660
Al	-2.41059000	9.78082000	2.20274000	2.48270490
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Al	0.00953000	5.58904000	2.20274000	2.48272180
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Al	4.84978000	5.58904000	2.20274000	2.48272840
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O	6.52853000	5.47588000	3.05515000	-1.64179850
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Al	9.69003000	2.79452000	3.90756000	2.47778360
Al	4.84978000	11.17808000	3.90756000	2.47773510
Al	0.00953000	2.79452000	3.90756000	2.47778430
Al	7.26991000	6.98630000	3.90756000	2.47773920
Al	-4.83072000	11.17808000	3.90756000	2.47793100
Al	-2.41059000	6.98630000	3.90756000	2.47791220
Al	4.84978000	2.79452000	3.90756000	2.47777650
Al	0.00953000	11.17808000	3.90756000	2.47786300
Al	2.42966000	6.98630000	3.90756000	2.47778940
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Al	-2.41059000	4.19178000	4.40548000	2.47232840
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Al	0.00953000	8.38356000	4.40548000	2.47247280
Al	2.42966000	4.19178000	4.40548000	2.47245480
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O	3.36702000	11.17808000	5.25789000	-1.64331100
O	5.59116000	12.46219000	5.25789000	-1.65406630
O	5.59116000	9.89398000	5.25789000	-1.64912200
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O	5.78715000	6.98630000	5.25789000	-1.64324680
O	8.01128000	8.27041000	5.25789000	-1.65415430
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Al	-2.41059000	6.98630000	6.60910000	2.47679750
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Al	0.00953000	11.17808000	6.60910000	2.47682650
Al	2.42966000	6.98630000	6.60910000	2.47703580
O	11.36395000	0.11351000	7.46570000	-1.64865280
O	11.37150000	2.68537000	7.46570000	-1.64974220
O	13.59502000	1.39291000	7.46570000	-1.65431530
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O	8.75477000	9.77647000	7.46570000	-1.65449540
O	1.68345000	0.11351000	7.46570000	-1.64980580
O	8.94383000	4.30529000	7.46570000	-1.64934400
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O	4.10358000	4.30529000	7.46570000	-1.64880320
O	4.11112000	6.87715000	7.46570000	-1.64895320
O	6.33465000	5.58469000	7.46570000	-1.65347940
Al	9.69003000	0.00000000	8.32833000	2.47084740
Al	4.84978000	8.38356000	8.32833000	2.47148540
Al	0.00954000	0.00000000	8.32833000	2.47178070
Al	7.26991000	4.19178000	8.32833000	2.47168010
Al	-4.83072000	8.38356000	8.32833000	2.47173100
Al	-2.41059000	4.19178000	8.32833000	2.47100450
Al	4.84978000	0.00000000	8.32833000	2.47205370
Al	0.00953000	8.38356000	8.32833000	2.47024460
Al	2.42966000	4.19178000	8.32833000	2.47166280
Al	12.11016000	1.39726000	8.78548000	2.47260980
Al	7.26991000	9.78082000	8.78548000	2.47229220
Al	9.69003000	5.58904000	8.78548000	2.47239950
Al	2.42966000	1.39726000	8.78548000	2.47221050
Al	-2.41059000	9.78082000	8.78548000	2.47204380
Al	7.26991000	1.39726000	8.78548000	2.47234750
Al	0.00953000	5.58904000	8.78548000	2.47592430
Al	2.42966000	9.78082000	8.78548000	2.47664790
Al	4.84978000	5.58904000	8.78548000	2.47619430
O	8.01661000	2.88194000	9.68989000	-1.64430060
O	3.17636000	11.26550000	9.68989000	-1.63713700
O	10.45104000	1.30159000	9.68989000	-1.65680810
O	12.85686000	2.88194000	9.68989000	-1.64165200
O	5.59648000	7.07372000	9.68989000	-1.63710270
O	5.61079000	9.68514000	9.68989000	-1.65688200
O	13.02257000	0.00826000	9.68989000	-1.66765540
O	8.01661000	11.26550000	9.68989000	-1.64435430
O	0.77054000	1.30159000	9.68989000	-1.66021740
O	8.03091000	5.49337000	9.68989000	-1.65873180
O	8.18232000	8.39182000	9.68989000	-1.66767430
O	3.17636000	2.88194000	9.68989000	-1.64384600
O	10.43673000	7.07372000	9.68989000	-1.64425130
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O	10.60245000	4.20004000	9.68989000	-1.66786180
O	3.34207000	0.00826000	9.68989000	-1.66954370
O	-1.66389000	11.26550000	9.68989000	-1.64248330

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O	-1.49818000	8.39182000	9.68989000	-1.66639010
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O	0.77054000	9.68514000	9.68989000	-1.64799750
O	0.92195000	4.20004000	9.68989000	-1.65799030
O	8.18232000	0.00827000	9.68989000	-1.66377900
O	3.19067000	5.49337000	9.68989000	-1.64499710
O	3.34207000	8.39182000	9.68989000	-1.65603370
O	5.76220000	4.20004000	9.68989000	-1.65543760
Al	9.69003000	2.79452000	10.71830000	2.47819320
Al	4.84978000	11.17808000	10.71830000	2.47551020
Al	0.00953000	2.79452000	10.71830000	2.47496700
Al	7.26991000	6.98630000	10.71830000	2.47991410
Al	-4.83072000	11.17808000	10.71830000	2.47571910
Al	-2.41059000	6.98630000	10.71830000	2.47453940
Al	4.84978000	2.79452000	10.71830000	2.47873460
Al	0.00953000	11.17808000	10.71830000	2.47954600
Al	2.42966000	6.98630000	10.71830000	3.00000000
Al	9.69003000	0.00000000	10.98601000	2.47130850
Al	4.84978000	8.38356000	10.98601000	2.46927120
Al	0.00954000	0.00000000	10.98601000	2.46993420
Al	7.26991000	4.19178000	10.98601000	2.47274220
Al	-4.83072000	8.38356000	10.98601000	2.46906800
Al	-2.41059000	4.19178000	10.98601000	2.47194180
Al	4.84978000	0.00000000	10.98601000	2.47093230
Al	0.00953000	8.38356000	10.98601000	2.47155930
Al	2.42966000	4.19178000	10.98601000	2.47090480
O	8.87185000	4.08919000	11.85246000	-1.62252030
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O	11.22060000	2.85590000	11.85265000	-1.62612410
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O	4.11165000	9.79568000	11.86778000	-1.60113620
O	6.37688000	11.23835000	11.85301000	-1.62800600
O	-0.80424000	4.09614000	11.84558000	-1.60592940
O	6.44971000	8.29571000	11.87028000	-1.63239660
O	-0.69787000	1.43613000	11.85291000	-1.62591400
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O	6.37652000	2.85357000	11.86063000	-1.62444230
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O	-0.81369000	12.46974000	11.85298000	-1.62132230
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O	1.54269000	11.23281000	11.84538000	-1.60857390
O	1.58140000	8.30753000	11.94203000	-1.57806190
O	1.70776000	5.58892000	11.95055000	-1.57463480
O	3.99756000	7.06003000	11.94655000	-1.57048290
Al	12.11154000	1.39918000	11.88304000	2.41520240
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Al	9.68720000	5.58938000	11.88369000	2.41518900
Al	2.43408000	1.37943000	11.86062000	2.41597990
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Al	7.27088000	1.39475000	11.88337000	2.41345420
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Pt	2.38607000	7.01776000	15.27519000	-0.53625490
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Pt	2.46667000	9.69709000	14.85473000	-0.77223970
Pt	4.70976000	5.61070000	14.86362000	-0.78947210
Sn	2.36336000	4.51417000	14.19239000	0.95029750
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Al	7.26991000	6.98630000	0.00000000	2.17054780
Al	-4.83072000	11.17808000	0.00000000	2.17061210
Al	-2.41059000	6.98630000	0.00000000	2.17040460
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O	10.62741000	1.39726000	0.85241000	-1.55161990
O	12.85153000	0.11316000	0.85241000	-1.55993110
O	12.85153000	2.68136000	0.85241000	-1.55767630
O	5.78716000	9.78082000	0.85241000	-1.55172600

O	8.01128000	8.49672000	0.85241000	-1.56008270
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O	0.94691000	1.39726000	0.85241000	-1.55179960
O	8.20728000	5.58904000	0.85241000	-1.55171000
O	10.43141000	4.30494000	0.85241000	-1.55995190
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O	8.01128000	2.68136000	0.85241000	-1.55774680
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O	3.17103000	8.49672000	0.85241000	-1.55987650
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Al	4.84978000	8.38356000	1.70482000	2.46338220
Al	0.00954000	0.00000000	1.70482000	2.46329000
Al	7.26991000	4.19178000	1.70482000	2.46330650
Al	-4.83072000	8.38356000	1.70482000	2.46327870
Al	-2.41059000	4.19178000	1.70482000	2.46327520
Al	4.84978000	0.00000000	1.70482000	2.46344640
Al	0.00953000	8.38356000	1.70482000	2.46328930
Al	2.42966000	4.19178000	1.70482000	2.46345880
Al	12.11016000	1.39726000	2.20274000	2.48273730
Al	7.26991000	9.78082000	2.20274000	2.48265030
Al	9.69003000	5.58904000	2.20274000	2.48269180
Al	2.42966000	1.39726000	2.20274000	2.48270370
Al	-2.41059000	9.78082000	2.20274000	2.48274730
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Al	0.00953000	5.58904000	2.20274000	2.48272660
Al	2.42966000	9.78082000	2.20274000	2.48275830
Al	4.84978000	5.58904000	2.20274000	2.48283140
O	8.94865000	1.28410000	3.05515000	-1.64149890
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O	4.10840000	9.66766000	3.05515000	-1.64148320
O	11.36879000	2.90768000	3.05515000	-1.64951900
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O	1.68828000	2.90768000	3.05515000	-1.64933680
O	-3.34797000	8.38357000	3.05515000	-1.62393180
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Al	0.00953000	2.79452000	3.90756000	2.47763170
Al	7.26991000	6.98630000	3.90756000	2.47767530
Al	-4.83072000	11.17808000	3.90756000	2.47780750
Al	-2.41059000	6.98630000	3.90756000	2.47759290
Al	4.84978000	2.79452000	3.90756000	2.47770820
Al	0.00953000	11.17808000	3.90756000	2.47754490
Al	2.42966000	6.98630000	3.90756000	2.47753440
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Al	4.84978000	8.38356000	4.40548000	2.47243820
Al	0.00954000	0.00000000	4.40548000	2.47242790
Al	7.26991000	4.19178000	4.40548000	2.47227380
Al	-4.83072000	8.38356000	4.40548000	2.47221770
Al	-2.41059000	4.19178000	4.40548000	2.47233530
Al	4.84978000	0.00000000	4.40548000	2.47238610
Al	0.00953000	8.38356000	4.40548000	2.47223140
Al	2.42966000	4.19178000	4.40548000	2.47238240

O	8.20728000	2.79452000	5.25789000	-1.64339840
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O	10.43142000	1.51042000	5.25789000	-1.64913650
O	3.36702000	11.17808000	5.25789000	-1.64309360
O	5.59116000	12.46219000	5.25789000	-1.65432650
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O	5.78715000	6.98630000	5.25789000	-1.64306800
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O	0.94690000	6.98630000	5.25789000	-1.64321490
O	3.17103000	8.27041000	5.25789000	-1.65413700
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Al	-2.41059000	9.78082000	6.11030000	2.47600210
Al	7.26991000	1.39726000	6.11030000	2.47593240
Al	0.00953000	5.58904000	6.11030000	2.47644060
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Al	4.84978000	5.58904000	6.11030000	2.47620460
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Al	0.00953000	2.79452000	6.60910000	2.47670070
Al	7.26991000	6.98630000	6.60910000	2.47695580
Al	-4.83072000	11.17808000	6.60910000	2.47681610
Al	-2.41059000	6.98630000	6.60910000	2.47686320
Al	4.84978000	2.79452000	6.60910000	2.47688580

Al	0.00953000	11.17808000	6.60910000	2.47697300
Al	2.42966000	6.98630000	6.60910000	2.47750040
O	11.36395000	0.11351000	7.46570000	-1.64864940
O	11.37150000	2.68537000	7.46570000	-1.64961010
O	13.59502000	1.39291000	7.46570000	-1.65417570
O	6.52370000	8.49707000	7.46570000	-1.64923410
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O	8.75477000	9.77647000	7.46570000	-1.65453810
O	1.68345000	0.11351000	7.46570000	-1.64983070
O	8.94383000	4.30529000	7.46570000	-1.64894450
O	8.95137000	6.87715000	7.46570000	-1.65009200
O	1.69100000	2.68537000	7.46570000	-1.64927960
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O	6.33465000	5.58469000	7.46570000	-1.65371960
Al	9.69003000	0.00000000	8.32833000	2.47039620
Al	4.84978000	8.38356000	8.32833000	2.47133560
Al	0.00954000	0.00000000	8.32833000	2.47207990
Al	7.26991000	4.19178000	8.32833000	2.47165350
Al	-4.83072000	8.38356000	8.32833000	2.47190400
Al	-2.41059000	4.19178000	8.32833000	2.47067970
Al	4.84978000	0.00000000	8.32833000	2.47243600
Al	0.00953000	8.38356000	8.32833000	2.46984300
Al	2.42966000	4.19178000	8.32833000	2.47101860
Al	12.11016000	1.39726000	8.78548000	2.47253760
Al	7.26991000	9.78082000	8.78548000	2.47202160
Al	9.69003000	5.58904000	8.78548000	2.47183390
Al	2.42966000	1.39726000	8.78548000	2.47232080
Al	-2.41059000	9.78082000	8.78548000	2.47116070

Al	7.26991000	1.39726000	8.78548000	2.47202520
Al	0.00953000	5.58904000	8.78548000	2.47522050
Al	2.42966000	9.78082000	8.78548000	2.47596360
Al	4.84978000	5.58904000	8.78548000	2.47695590
O	8.01661000	2.88194000	9.68989000	-1.64440720
O	3.17636000	11.26550000	9.68989000	-1.63911330
O	10.45104000	1.30159000	9.68989000	-1.65577450
O	12.85686000	2.88194000	9.68989000	-1.64182460
O	5.59648000	7.07372000	9.68989000	-1.63649280
O	5.61079000	9.68514000	9.68989000	-1.65779750
O	13.02257000	0.00826000	9.68989000	-1.66693320
O	8.01661000	11.26550000	9.68989000	-1.64473360
O	0.77054000	1.30159000	9.68989000	-1.66063170
O	8.03091000	5.49337000	9.68989000	-1.65966130
O	8.18232000	8.39182000	9.68989000	-1.66652510
O	3.17636000	2.88194000	9.68989000	-1.64372940
O	10.43673000	7.07372000	9.68989000	-1.64571330
O	-4.06971000	9.68514000	9.68989000	-1.66093320
O	10.60245000	4.20004000	9.68989000	-1.66773040
O	3.34207000	0.00826000	9.68989000	-1.66868280
O	-1.66389000	11.26550000	9.68989000	-1.64293290
O	-1.64958000	5.49336000	9.68989000	-1.64717430
O	5.61079000	1.30159000	9.68989000	-1.66044740
O	-1.49818000	8.39182000	9.68989000	-1.66314160
O	0.75623000	7.07372000	9.68989000	-1.63729920
O	0.77054000	9.68514000	9.68989000	-1.64718930
O	0.92195000	4.20004000	9.68989000	-1.65665570
O	8.18232000	0.00827000	9.68989000	-1.66431030
O	3.19067000	5.49337000	9.68989000	-1.64970320
O	3.34207000	8.39182000	9.68989000	-1.65309410
O	5.76220000	4.20004000	9.68989000	-1.65675010
Al	9.69003000	2.79452000	10.71830000	2.47805830
Al	4.84978000	11.17808000	10.71830000	2.48145050
Al	0.00953000	2.79452000	10.71830000	2.47718040
Al	7.26991000	6.98630000	10.71830000	2.47283240
Al	-4.83072000	11.17808000	10.71830000	2.47690580
Al	-2.41059000	6.98630000	10.71830000	2.47554150
Al	4.84978000	2.79452000	10.71830000	2.47952890
Al	0.00953000	11.17808000	10.71830000	2.47557890
Al	2.42966000	6.98630000	10.71830000	2.47665850
Al	9.69003000	0.00000000	10.98601000	2.47230230
Al	4.84978000	8.38356000	10.98601000	2.46871180
Al	0.00954000	0.00000000	10.98601000	2.46945380

Al	7.26991000	4.19178000	10.98601000	2.47070770
Al	-4.83072000	8.38356000	10.98601000	2.47067490
Al	-2.41059000	4.19178000	10.98601000	2.47223780
Al	4.84978000	0.00000000	10.98601000	2.47071380
Al	0.00953000	8.38356000	10.98601000	2.47008030
Al	2.42966000	4.19178000	10.98601000	2.47318860
O	8.86970000	4.09141000	11.85311000	-1.62262620
O	8.97676000	1.43895000	11.85276000	-1.62289780
O	11.21824000	2.86002000	11.85342000	-1.62441380
O	4.03688000	12.47866000	11.85889000	-1.62322670
O	4.13482000	9.80564000	11.86298000	-1.61456640
O	6.37759000	11.25083000	11.85663000	-1.62601140
O	-0.80606000	4.10886000	11.84753000	-1.61667370
O	6.43875000	8.29823000	11.94190000	-1.60035790
O	-0.69816000	1.43753000	11.85179000	-1.62457870
O	6.56729000	5.64457000	11.83039000	-1.61013950
O	8.79263000	7.05981000	11.85864000	-1.62464870
O	1.54969000	2.85676000	11.87136000	-1.62557210
O	-5.65043000	12.46695000	11.85041000	-1.62021730
O	-5.53375000	9.81932000	11.85151000	-1.62295380
O	-3.30863000	11.24648000	11.84872000	-1.62479090
O	-3.23656000	8.27701000	11.85448000	-1.62668710
O	4.03050000	4.11566000	11.85478000	-1.61447590
O	-3.12838000	5.63786000	11.85728000	-1.62496850
O	4.13822000	1.43514000	11.85315000	-1.62348520
O	6.38128000	2.85351000	11.86081000	-1.62360950
O	-0.86843000	7.05479000	11.85576000	-1.60035440
O	-0.81375000	12.46382000	11.85299000	-1.62209110
O	-0.72383000	9.80212000	11.89477000	-1.61581370
O	1.55387000	11.21073000	11.83318000	-1.60737820
O	1.57548000	8.30897000	11.93256000	-1.58044610
O	1.69878000	5.60197000	11.97330000	-1.55484860
O	3.98290000	7.00531000	11.81788000	-1.60972330
Al	12.11187000	1.40442000	11.89349000	2.41599800
Al	7.28749000	9.82051000	11.87565000	2.40771290
Al	9.68425000	5.59070000	11.87037000	2.41545980
Al	2.43094000	1.39212000	11.87656000	2.41466140
Al	-2.44206000	9.78323000	11.83294000	2.41114100
Al	7.27049000	1.39121000	11.87727000	2.41381840
Al	-0.07181000	5.58261000	12.40301000	2.38394460
Al	2.45835000	9.80724000	12.40385000	2.38404220
Al	4.89369000	5.57635000	12.29765000	2.37736470
Pt	2.09521000	9.85435000	14.84548000	-0.74734980

Pt	3.45147000	7.76779000	14.93777000	-0.40237310
Pt	5.05299000	5.72232000	14.77545000	-0.77597270
Pt	0.08749000	6.01712000	14.83133000	-0.94579510
Sn	2.43612000	5.24433000	14.22320000	0.95677460
Sn	5.94877000	8.13991000	14.34715000	0.87119180
Sn	0.00926000	8.53457000	14.18874000	0.97334610

Figure S5

Coordinates for ethylene binding Pt_4Sn_3 on alumina, the format is

Number of atom

Comment line: ethylene-cluster-support-isomer

symbol x y z bader_charge

283				
c2h4-pt4sn3-al2o3-C				
Al	-4.83072000	11.17808000	0.00000000	2.16835670
Al	-2.41059000	6.98630000	0.00000000	2.16836610
Al	0.00953000	11.17808000	0.00000000	2.16828320
Al	0.00953000	2.79452000	0.00000000	2.16835890
Al	2.42966000	6.98630000	0.00000000	2.16821110
Al	4.84978000	2.79452000	0.00000000	2.16810560
Al	4.84978000	11.17808000	0.00000000	2.16840470
Al	7.26991000	6.98630000	0.00000000	2.16822290
Al	9.69003000	2.79452000	0.00000000	2.16838310
O	-3.89334000	9.78082000	0.85241000	-1.55250690
O	-1.66922000	8.49672000	0.85241000	-1.56094690
O	-1.66922000	11.06492000	0.85241000	-1.55851860
O	-1.47322000	5.58904000	0.85241000	-1.55261790
O	0.75091000	4.30494000	0.85241000	-1.56100260
O	0.75091000	6.87314000	0.85241000	-1.55860270
O	0.94691000	9.78082000	0.85241000	-1.55254850
O	0.94691000	1.39726000	0.85241000	-1.55256960
O	3.17104000	0.11316000	0.85241000	-1.56089930
O	3.17103000	8.49672000	0.85241000	-1.56066150
O	3.17103000	2.68136000	0.85241000	-1.55857680
O	3.17103000	11.06492000	0.85241000	-1.55852860
O	3.36703000	5.58904000	0.85241000	-1.55248500
O	5.59116000	4.30494000	0.85241000	-1.56091090
O	5.59116000	6.87314000	0.85241000	-1.55844860
O	5.78716000	1.39726000	0.85241000	-1.55253210
O	5.78716000	9.78082000	0.85241000	-1.55243210
O	8.01128000	8.49672000	0.85241000	-1.56089220
O	8.01128000	0.11316000	0.85241000	-1.56091470
O	8.01128000	2.68136000	0.85241000	-1.55859830
O	8.01128000	11.06492000	0.85241000	-1.55856600
O	8.20728000	5.58904000	0.85241000	-1.55249750
O	10.43141000	4.30494000	0.85241000	-1.56108960
O	10.43141000	6.87314000	0.85241000	-1.55861420

O	10.62741000	1.39726000	0.85241000	-1.55259440
O	12.85153000	0.11316000	0.85241000	-1.56087530
O	12.85153000	2.68136000	0.85241000	-1.55877710
Al	-4.83072000	8.38356000	1.70482000	2.46345100
Al	-2.41059000	4.19178000	1.70482000	2.46338040
Al	0.00953000	8.38356000	1.70482000	2.46357470
Al	0.00954000	0.00000000	1.70482000	2.46338380
Al	2.42966000	4.19178000	1.70482000	2.46356770
Al	4.84978000	0.00000000	1.70482000	2.46343960
Al	4.84978000	8.38356000	1.70482000	2.46322890
Al	7.26991000	4.19178000	1.70482000	2.46343730
Al	9.69003000	0.00000000	1.70482000	2.46339910
Al	-2.41059000	9.78082000	2.20274000	2.48276420
Al	0.00953000	5.58904000	2.20274000	2.48269530
Al	2.42966000	1.39726000	2.20274000	2.48278940
Al	2.42966000	9.78082000	2.20274000	2.48280320
Al	4.84978000	5.58904000	2.20274000	2.48284570
Al	7.26991000	9.78082000	2.20274000	2.48284850
Al	7.26991000	1.39726000	2.20274000	2.48276560
Al	9.69003000	5.58904000	2.20274000	2.48270170
Al	12.11016000	1.39726000	2.20274000	2.48272260
O	-5.57210000	9.66766000	3.05515000	-1.64219710
O	-3.34796000	8.38356000	3.05515000	-1.62429430
O	-3.15197000	5.47588000	3.05515000	-1.64221710
O	-3.15197000	11.29124000	3.05515000	-1.65010920
O	-0.92784000	4.19178000	3.05515000	-1.62439080
O	-0.73185000	1.28410000	3.05515000	-1.64241950
O	-0.73185000	9.66766000	3.05515000	-1.64230560
O	-0.73184000	7.09945000	3.05515000	-1.65023570
O	1.49229000	8.38356000	3.05515000	-1.62428300
O	1.49229000	0.00001000	3.05515000	-1.62422990
O	1.68828000	5.47588000	3.05515000	-1.64229550
O	1.68828000	2.90768000	3.05515000	-1.65008330
O	1.68828000	11.29123000	3.05515000	-1.65007540
O	3.91241000	4.19178000	3.05515000	-1.62432390
O	4.10840000	9.66766000	3.05515000	-1.64210320
O	4.10840000	1.28410000	3.05515000	-1.64230500
O	4.10841000	7.09946000	3.05515000	-1.64997940
O	6.33254000	0.00001000	3.05515000	-1.62434370
O	6.33254000	8.38356000	3.05515000	-1.62410060
O	6.52853000	11.29123000	3.05515000	-1.64991690
O	6.52853000	5.47588000	3.05515000	-1.64202000
O	6.52853000	2.90768000	3.05515000	-1.65023850

O	8.75266000	4.19178000	3.05515000	-1.62432400
O	8.94866000	7.09945000	3.05515000	-1.65014920
O	8.94865000	1.28410000	3.05515000	-1.64230910
O	11.17277000	0.00000000	3.05515000	-1.62419920
O	11.36878000	2.90767000	3.05515000	-1.65025400
Al	-4.83072000	11.17808000	3.90756000	2.47791210
Al	-2.41059000	6.98630000	3.90756000	2.47798410
Al	0.00953000	11.17808000	3.90756000	2.47797380
Al	0.00953000	2.79452000	3.90756000	2.47801970
Al	2.42966000	6.98630000	3.90756000	2.47792060
Al	4.84978000	2.79452000	3.90756000	2.47799510
Al	4.84978000	11.17808000	3.90756000	2.47795600
Al	7.26991000	6.98630000	3.90756000	2.47779550
Al	9.69003000	2.79452000	3.90756000	2.47805510
Al	-4.83072000	8.38356000	4.40548000	2.47237860
Al	-2.41059000	4.19178000	4.40548000	2.47222220
Al	0.00953000	8.38356000	4.40548000	2.47238060
Al	0.00954000	0.00000000	4.40548000	2.47235200
Al	2.42966000	4.19178000	4.40548000	2.47229410
Al	4.84978000	0.00000000	4.40548000	2.47249800
Al	4.84978000	8.38356000	4.40548000	2.47230640
Al	7.26991000	4.19178000	4.40548000	2.47237240
Al	9.69003000	0.00000000	4.40548000	2.47221490
O	-6.31347000	11.17808000	5.25789000	-1.64346670
O	-4.08934000	12.46219000	5.25789000	-1.65402070
O	-4.08934000	9.89398000	5.25789000	-1.64905620
O	-3.89335000	6.98630000	5.25789000	-1.64353540
O	-1.66922000	8.27040000	5.25789000	-1.65377440
O	-1.66921000	5.70219000	5.25789000	-1.64895890
O	-1.47322000	11.17808000	5.25789000	-1.64356100
O	-1.47323000	2.79452000	5.25789000	-1.64332600
O	0.75091000	4.07862000	5.25789000	-1.65391280
O	0.75091000	12.46219000	5.25789000	-1.65394680
O	0.75091000	9.89397000	5.25789000	-1.64894110
O	0.75091000	1.51042000	5.25789000	-1.64888330
O	0.94690000	6.98630000	5.25789000	-1.64348210
O	3.17103000	8.27040000	5.25789000	-1.65375600
O	3.17104000	5.70220000	5.25789000	-1.64899350
O	3.36703000	2.79452000	5.25789000	-1.64346170
O	3.36702000	11.17808000	5.25789000	-1.64350340
O	5.59116000	12.46219000	5.25789000	-1.65415290
O	5.59116000	4.07863000	5.25789000	-1.65393650
O	5.59116000	9.89397000	5.25789000	-1.64917700

O	5.59116000	1.51042000	5.25789000	-1.64897800
O	5.78715000	6.98630000	5.25789000	-1.64332560
O	8.01128000	8.27040000	5.25789000	-1.65398360
O	8.01129000	5.70219000	5.25789000	-1.64920210
O	8.20727000	2.79452000	5.25789000	-1.64321350
O	10.43141000	4.07862000	5.25789000	-1.65398640
O	10.43141000	1.51041000	5.25789000	-1.64891360
Al	-2.41059000	9.78082000	6.11030000	2.47602860
Al	0.00953000	5.58904000	6.11030000	2.47587930
Al	2.42966000	1.39726000	6.11030000	2.47605400
Al	2.42966000	9.78082000	6.11030000	2.47611990
Al	4.84978000	5.58904000	6.11030000	2.47614150
Al	7.26991000	9.78082000	6.11030000	2.47625480
Al	7.26991000	1.39726000	6.11030000	2.47605260
Al	9.69003000	5.58904000	6.11030000	2.47623650
Al	12.11016000	1.39726000	6.11030000	2.47597870
Al	-4.83072000	11.17808000	6.60910000	2.47666500
Al	-2.41059000	6.98630000	6.60910000	2.47689680
Al	0.00953000	11.17808000	6.60910000	2.47667310
Al	0.00953000	2.79452000	6.60910000	2.47665370
Al	2.42966000	6.98630000	6.60910000	2.47697370
Al	4.84978000	2.79452000	6.60910000	2.47678850
Al	4.84978000	11.17808000	6.60910000	2.47683960
Al	7.26991000	6.98630000	6.60910000	2.47681010
Al	9.69003000	2.79452000	6.60910000	2.47677220
O	-3.15680000	8.49706000	7.46570000	-1.64971450
O	-3.14925000	11.06893000	7.46570000	-1.64973520
O	-0.92572000	9.77647000	7.46570000	-1.65382810
O	-0.73667000	4.30528000	7.46570000	-1.64992110
O	-0.72913000	6.87715000	7.46570000	-1.64998140
O	1.49440000	5.58469000	7.46570000	-1.65360050
O	1.68345000	8.49706000	7.46570000	-1.64926620
O	1.68345000	0.11351000	7.46570000	-1.64901840
O	1.69100000	2.68537000	7.46570000	-1.65041430
O	1.69100000	11.06893000	7.46570000	-1.64922490
O	3.91453000	1.39291000	7.46570000	-1.65400640
O	3.91452000	9.77646000	7.46570000	-1.65342680
O	4.10358000	4.30528000	7.46570000	-1.64899290
O	4.11112000	6.87715000	7.46570000	-1.64912730
O	6.33465000	5.58468000	7.46570000	-1.65365090
O	6.52370000	0.11351000	7.46570000	-1.64895180
O	6.52370000	8.49706000	7.46570000	-1.64844190
O	6.53125000	2.68537000	7.46570000	-1.64971300

O	6.53125000	11.06893000	7.46570000	-1.64944500
O	8.75477000	9.77646000	7.46570000	-1.65344530
O	8.75477000	1.39291000	7.46570000	-1.65457100
O	8.94383000	4.30528000	7.46570000	-1.64980480
O	8.95137000	6.87715000	7.46570000	-1.64943930
O	11.17490000	5.58468000	7.46570000	-1.65457140
O	11.36395000	0.11351000	7.46570000	-1.64899970
O	11.37149000	2.68537000	7.46570000	-1.65022040
O	13.59502000	1.39291000	7.46570000	-1.65374160
Al	-4.83072000	8.38356000	8.32833000	2.47237380
Al	-2.41059000	4.19178000	8.32833000	2.47238080
Al	0.00953000	8.38356000	8.32833000	2.47085040
Al	0.00954000	0.00000000	8.32833000	2.47114120
Al	2.42966000	4.19178000	8.32833000	2.47076310
Al	4.84978000	0.00000000	8.32833000	2.47163270
Al	4.84978000	8.38356000	8.32833000	2.47063110
Al	7.26991000	4.19178000	8.32833000	2.47180120
Al	9.69003000	0.00000000	8.32833000	2.47133460
Al	-2.41059000	9.78082000	8.78548000	2.47248270
Al	0.00953000	5.58904000	8.78548000	2.47209060
Al	2.42966000	1.39726000	8.78548000	2.47248330
Al	2.42966000	9.78082000	8.78548000	2.47616250
Al	4.84978000	5.58904000	8.78548000	2.47657030
Al	7.26991000	9.78082000	8.78548000	2.47640750
Al	7.26991000	1.39726000	8.78548000	2.47196760
Al	9.69003000	5.58904000	8.78548000	2.47218070
Al	12.11016000	1.39726000	8.78548000	2.47150020
O	8.01661000	11.26550000	9.68989000	-1.64659600
O	10.43673000	7.07371000	9.68989000	-1.64291100
O	-4.06971000	9.68514000	9.68989000	-1.65987410
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O	-1.64959000	5.49336000	9.68989000	-1.66085470
O	-1.49818000	8.39182000	9.68989000	-1.66822640
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O	0.77054000	9.68514000	9.68989000	-1.64582140
O	0.77054000	1.30159000	9.68989000	-1.65671930
O	0.92195000	4.20004000	9.68989000	-1.66715650
O	3.17636000	11.26550000	9.68989000	-1.63903260
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O	3.34208000	0.00826000	9.68989000	-1.66818120
O	3.34207000	8.39182000	9.68989000	-1.65511170

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O	5.61079000	9.68514000	9.68989000	-1.64568960
O	5.76220000	4.20004000	9.68989000	-1.65404800
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O	8.03091000	5.49336000	9.68989000	-1.66111320
O	8.18232000	0.00826000	9.68989000	-1.66560390
O	8.18232000	8.39182000	9.68989000	-1.65666420
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Al	-2.41059000	6.98630000	10.71830000	2.47478550
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Al	0.00953000	2.79452000	10.71830000	2.47774100
Al	2.42966000	6.98630000	10.71830000	2.47890690
Al	4.84978000	2.79452000	10.71830000	2.47547900
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Al	9.69003000	2.79452000	10.71830000	2.47565990
Al	-4.83072000	8.38356000	10.98601000	2.47167240
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Al	0.00954000	0.00000000	10.98601000	2.47277390
Al	2.42966000	4.19178000	10.98601000	2.47221560
Al	4.84978000	0.00000000	10.98601000	2.47181200
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Al	7.26991000	4.19178000	10.98601000	2.47218640
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283				
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Al	2.42965000	12.57534000	1.70482000	2.46337970
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Al	2.42966000	1.39726000	2.20274000	2.48284090
Al	2.42966000	9.78082000	2.20274000	2.48270000

Al	4.84978000	5.58904000	2.20274000	2.48285270
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Al	-2.41059000	9.78082000	6.11030000	2.47610240
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Al	-4.83072000	11.17808000	6.60910000	2.47674510
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O	1.68345000	8.49706000	7.46570000	-1.64887040
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Al	-2.41059000	9.78082000	8.78548000	2.47219950
Al	0.00953000	5.58904000	8.78548000	2.47625090
Al	2.42966000	1.39726000	8.78548000	2.47640840
Al	2.42966000	9.78082000	8.78548000	2.47194270
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Al	9.69003000	5.58904000	8.78548000	2.47195780
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O	8.01661000	11.26550000	9.68989000	-1.64437140
O	10.43673000	7.07371000	9.68989000	-1.64280570
O	-4.06971000	9.68514000	9.68989000	-1.65984980
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O	12.85686000	2.88194000	9.68989000	-1.64356240
O	-1.64959000	5.49336000	9.68989000	-1.64558050
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O	0.75624000	7.07372000	9.68989000	-1.63734260
O	0.77054000	9.68514000	9.68989000	-1.65676890
O	0.77054000	1.30159000	9.68989000	-1.64806310
O	0.92195000	4.20004000	9.68989000	-1.65603580
O	3.17636000	11.26550000	9.68989000	-1.64541210
O	3.17636000	2.88194000	9.68989000	-1.63233310
O	3.19067000	5.49336000	9.68989000	-1.64584510
O	3.34208000	0.00826000	9.68989000	-1.65427810
O	3.34207000	8.39182000	9.68989000	-1.66027020
O	5.59648000	7.07372000	9.68989000	-1.64235140
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O	5.61079000	9.68514000	9.68989000	-1.65684430
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O	8.03091000	5.49336000	9.68989000	-1.66094150
O	8.18232000	0.00826000	9.68989000	-1.66878640
O	8.18232000	8.39182000	9.68989000	-1.66845090
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Al	-4.83072000	11.17808000	10.71830000	2.47562190
Al	-2.41059000	6.98630000	10.71830000	2.48018870
Al	0.00953000	11.17808000	10.71830000	2.47565310
Al	0.00953000	2.79452000	10.71830000	2.47712740
Al	2.42966000	6.98630000	10.71830000	2.47827230

Al	4.84978000	2.79452000	10.71830000	2.47996500
Al	4.84978000	11.17808000	10.71830000	2.47784450
Al	7.26991000	6.98630000	10.71830000	2.48093340
Al	9.69003000	2.79452000	10.71830000	2.47509870
Al	-4.83072000	8.38356000	10.98601000	2.47262440
Al	-2.41059000	4.19178000	10.98601000	2.47103660
Al	0.00953000	8.38356000	10.98601000	2.46922110
Al	-7.25084000	12.57534000	10.98601000	2.47134900
Al	2.42966000	4.19178000	10.98601000	2.47322500
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Al	4.84978000	8.38356000	10.98601000	2.47355290
Al	7.26991000	4.19178000	10.98601000	2.47153260
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Al	2.43332000	9.80555000	11.86199000	2.41741520
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Al	7.27433000	9.79305000	11.86418000	2.41745340
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C	7.04475000	5.97873000	15.16949000	-0.19234150
C	6.34041000	7.20083000	15.14689000	-0.21185610
H	7.35445000	5.53311000	16.12066000	0.09224840
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Al	0.00953000	2.79452000	0.00000000	2.16872940
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O	0.94691000	9.78082000	0.85241000	-1.55218610
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Al	4.84978000	0.00000000	1.70482000	2.46333930
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Al	7.26991000	4.19178000	1.70482000	2.46337030
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Al	2.42966000	1.39726000	2.20274000	2.48271280
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Al	0.00953000	11.17808000	3.90756000	2.47802710
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Al	4.84978000	2.79452000	3.90756000	2.47777930
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O	3.17103000	8.27040000	5.25789000	-1.65424240
O	3.17104000	5.70220000	5.25789000	-1.64895180
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Al	2.42966000	1.39726000	6.11030000	2.47629230
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O	1.68345000	8.49706000	7.46570000	-1.64840790

O	1.68345000	0.11351000	7.46570000	-1.64900090
O	1.69100000	2.68537000	7.46570000	-1.64882790
O	1.69100000	11.06893000	7.46570000	-1.64997540
O	3.91453000	1.39291000	7.46570000	-1.65364040
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O	4.10358000	4.30528000	7.46570000	-1.64858320
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Al	2.42966000	1.39726000	8.78548000	2.47641370
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Al	9.69003000	5.58904000	8.78548000	2.47201320
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O	10.43673000	7.07371000	9.68989000	-1.64334880
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O	3.17636000	2.88194000	9.68989000	-1.63386150
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O	3.34207000	8.39182000	9.68989000	-1.66318640
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Al	-2.41059000	6.98630000	10.71830000	2.47953330
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Al	0.00953000	2.79452000	10.71830000	2.47726800
Al	2.42966000	6.98630000	10.71830000	2.47684890
Al	4.84978000	2.79452000	10.71830000	2.47772760
Al	4.84978000	11.17808000	10.71830000	2.47650890
Al	7.26991000	6.98630000	10.71830000	2.48016510
Al	9.69003000	2.79452000	10.71830000	2.47320640
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Al	-2.41059000	4.19178000	10.98601000	2.47150890
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Al	4.84978000	0.00000000	10.98601000	2.47290330
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Al	2.42966000	1.39726000	6.11030000	2.47611470
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O	13.59502000	1.39291000	7.46570000	-1.65363240
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O	-4.06971000	9.68514000	9.68989000	-1.66057590
O	-1.66389000	11.26550000	9.68989000	-1.64386500
O	12.85686000	2.88194000	9.68989000	-1.64606360
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O	-1.49818000	8.39182000	9.68989000	-1.66835060
O	0.75624000	7.07372000	9.68989000	-1.64352320
O	0.77054000	9.68514000	9.68989000	-1.64657080
O	0.77054000	1.30159000	9.68989000	-1.65625800
O	0.92195000	4.20004000	9.68989000	-1.66853790
O	3.17636000	11.26550000	9.68989000	-1.63973980
O	3.17636000	2.88194000	9.68989000	-1.64287440
O	3.19067000	5.49336000	9.68989000	-1.64775960
O	3.34208000	0.00826000	9.68989000	-1.66835630
O	3.34207000	8.39182000	9.68989000	-1.65614370
O	5.59648000	7.07372000	9.68989000	-1.63055990
O	5.61079000	1.30159000	9.68989000	-1.65943280
O	5.61079000	9.68514000	9.68989000	-1.64768510
O	5.76220000	4.20004000	9.68989000	-1.65553120
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Al	0.00953000	2.79452000	10.71830000	2.47800300
Al	2.42966000	6.98630000	10.71830000	2.47716630
Al	4.84978000	2.79452000	10.71830000	2.47540840
Al	4.84978000	11.17808000	10.71830000	2.47813800
Al	7.26991000	6.98630000	10.71830000	2.47658330
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Al	-4.83072000	8.38356000	10.98601000	2.46933270
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Al	2.42966000	4.19178000	10.98601000	2.47257150
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O	3.36703000	5.58904000	0.85241000	-1.55315520
O	5.59116000	4.30494000	0.85241000	-1.56164190
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Al	0.00953000	8.38356000	1.70482000	2.46342850
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O	1.69100000	11.06893000	7.46570000	-1.65045870
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Al	2.42966000	1.39726000	8.78548000	2.47672220

Al	2.42966000	9.78082000	8.78548000	2.47118220
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O	12.85686000	2.88194000	9.68989000	-1.64447220
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O	0.77054000	9.68514000	9.68989000	-1.65813500
O	0.77054000	1.30159000	9.68989000	-1.64802440
O	0.92195000	4.20004000	9.68989000	-1.65678060
O	3.17636000	11.26550000	9.68989000	-1.64520040
O	3.17636000	2.88194000	9.68989000	-1.63269410
O	3.19067000	5.49336000	9.68989000	-1.64598810
O	3.34208000	0.00826000	9.68989000	-1.65287890
O	3.34207000	8.39182000	9.68989000	-1.65784260
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O	5.61079000	9.68514000	9.68989000	-1.65598210
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O	8.01661000	2.88194000	9.68989000	-1.64414860
O	8.03091000	5.49336000	9.68989000	-1.65971710
O	8.18232000	0.00826000	9.68989000	-1.67090910
O	8.18232000	8.39182000	9.68989000	-1.66707680
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Al	-2.41059000	6.98630000	10.71830000	2.48066230
Al	0.00953000	11.17808000	10.71830000	2.47588240
Al	0.00953000	2.79452000	10.71830000	2.47789410
Al	2.42966000	6.98630000	10.71830000	2.47742340
Al	4.84978000	2.79452000	10.71830000	2.47783490
Al	4.84978000	11.17808000	10.71830000	2.47778010
Al	7.26991000	6.98630000	10.71830000	2.48149050
Al	9.69003000	2.79452000	10.71830000	2.47493000
Al	-4.83072000	8.38356000	10.98601000	2.47188580

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Al	2.42966000	4.19178000	10.98601000	2.46980040
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283				
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Al	4.84978000	2.79452000	0.00000000	2.17016310
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Al	2.42966000	4.19178000	1.70482000	2.46345620
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Al	4.84978000	8.38356000	1.70482000	2.46338160
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Al	0.00953000	5.58904000	2.20274000	2.48280960
Al	2.42966000	1.39726000	2.20274000	2.48270590
Al	2.42966000	9.78082000	2.20274000	2.48272350
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Al	-2.41059000	6.98630000	3.90756000	2.47766280
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Al	0.00953000	2.79452000	3.90756000	2.47785160
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Al	0.00953000	11.17808000	6.60910000	2.47717280
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Al	4.84978000	2.79452000	6.60910000	2.47662340
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O	0.75624000	7.07372000	9.68989000	-1.64200590
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Al	2.42966000	6.98630000	10.71830000	2.47487510
Al	4.84978000	2.79452000	10.71830000	2.46989710
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Al	7.26991000	6.98630000	10.71830000	2.47852860
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Al	4.84978000	0.00000000	1.70482000	2.46328910
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O	3.19067000	5.49336000	9.68989000	-1.64510620
O	3.34208000	0.00826000	9.68989000	-1.65560010
O	3.34207000	8.39182000	9.68989000	-1.65661380
O	5.59648000	7.07372000	9.68989000	-1.64636530
O	5.61079000	1.30159000	9.68989000	-1.65941590
O	5.61079000	9.68514000	9.68989000	-1.65659980
O	5.76220000	4.20004000	9.68989000	-1.65463030
O	8.01661000	2.88194000	9.68989000	-1.64408590
O	8.03091000	5.49336000	9.68989000	-1.65967520
O	8.18232000	0.00826000	9.68989000	-1.66628340
O	8.18232000	8.39182000	9.68989000	-1.66803720
O	10.45104000	1.30158000	9.68989000	-1.66390420
O	10.60245000	4.20004000	9.68989000	-1.66844750

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Al	-4.83072000	11.17808000	10.71830000	2.47868740
Al	-2.41059000	6.98630000	10.71830000	2.47996860
Al	0.00953000	11.17808000	10.71830000	2.47691720
Al	0.00953000	2.79452000	10.71830000	2.47658540
Al	2.42966000	6.98630000	10.71830000	2.47820730
Al	4.84978000	2.79452000	10.71830000	2.47891200
Al	4.84978000	11.17808000	10.71830000	2.47382300
Al	7.26991000	6.98630000	10.71830000	2.47919020
Al	9.69003000	2.79452000	10.71830000	2.47365720
Al	-4.83072000	8.38356000	10.98601000	2.47090780
Al	-2.41059000	4.19178000	10.98601000	2.47154750
Al	0.00953000	8.38356000	10.98601000	2.47207660
Al	0.00954000	0.00000000	10.98601000	2.46890800
Al	2.42966000	4.19178000	10.98601000	2.47293080
Al	4.84978000	0.00000000	10.98601000	2.47409460
Al	4.84978000	8.38356000	10.98601000	2.47315260
Al	7.26991000	4.19178000	10.98601000	2.47195380
Al	9.69003000	0.00000000	10.98601000	2.46937450
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O	-5.54237000	9.82726000	11.85026000	-1.61958540
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O	11.22500000	2.85878000	11.85040000	-1.62853360
Al	-2.40618000	9.77938000	11.89425000	2.41724650
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Al	2.43232000	9.79371000	11.85173000	2.41487800
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Al	12.06002000	1.38004000	11.77006000	2.41173920
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C	5.65275000	7.94426000	15.22913000	-0.22745690
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283				
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Al	0.00953000	2.79452000	0.00000000	2.17025540
Al	2.42966000	6.98630000	0.00000000	2.17013200
Al	4.84978000	2.79452000	0.00000000	2.17001160
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O	0.94691000	9.78082000	0.85241000	-1.55188100

O	0.94691000	1.39726000	0.85241000	-1.55177160
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O	5.59116000	4.30494000	0.85241000	-1.55996320
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O	10.43141000	6.87314000	0.85241000	-1.55787700
O	10.62741000	1.39726000	0.85241000	-1.55191370
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Al	0.00953000	8.38356000	1.70482000	2.46328150
Al	0.00954000	0.00000000	1.70482000	2.46334070
Al	2.42966000	4.19178000	1.70482000	2.46333680
Al	4.84978000	0.00000000	1.70482000	2.46328950
Al	4.84978000	8.38356000	1.70482000	2.46331120
Al	7.26991000	4.19178000	1.70482000	2.46332000
Al	9.69003000	0.00000000	1.70482000	2.46324090
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Al	0.00953000	5.58904000	2.20274000	2.48281570
Al	2.42966000	1.39726000	2.20274000	2.48282250
Al	2.42966000	9.78082000	2.20274000	2.48265430
Al	4.84978000	5.58904000	2.20274000	2.48272840
Al	7.26991000	9.78082000	2.20274000	2.48263070
Al	7.26991000	1.39726000	2.20274000	2.48273820
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Al	-4.83072000	11.17808000	3.90756000	2.47772460
Al	-2.41059000	6.98630000	3.90756000	2.47776990
Al	0.00953000	11.17808000	3.90756000	2.47770270
Al	0.00953000	2.79452000	3.90756000	2.47773930
Al	2.42966000	6.98630000	3.90756000	2.47761910
Al	4.84978000	2.79452000	3.90756000	2.47755920
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O	3.17104000	5.70220000	5.25789000	-1.64902710
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O	10.43141000	1.51041000	5.25789000	-1.64904530
Al	-2.41059000	9.78082000	6.11030000	2.47623550
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Al	2.42966000	1.39726000	6.11030000	2.47635950
Al	2.42966000	9.78082000	6.11030000	2.47619830
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Al	-2.41059000	6.98630000	6.60910000	2.47683240
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Al	2.42966000	6.98630000	6.60910000	2.47715960
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Al	0.00953000	5.58904000	8.78548000	2.47589940
Al	2.42966000	1.39726000	8.78548000	2.47582620
Al	2.42966000	9.78082000	8.78548000	2.47178130
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Al	7.26991000	9.78082000	8.78548000	2.47203680
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O	-1.66389000	11.26550000	9.68989000	-1.64378970
O	12.85686000	2.88194000	9.68989000	-1.64555080
O	-1.64959000	5.49336000	9.68989000	-1.64595750
O	-1.49818000	8.39182000	9.68989000	-1.66435650
O	0.75624000	7.07372000	9.68989000	-1.63791210
O	0.77054000	9.68514000	9.68989000	-1.65742510
O	0.77054000	1.30159000	9.68989000	-1.64767330
O	0.92195000	4.20004000	9.68989000	-1.65630790
O	3.17636000	11.26550000	9.68989000	-1.64596440
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O	5.76220000	4.20004000	9.68989000	-1.65399410
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O	8.03091000	5.49336000	9.68989000	-1.66005370
O	8.18232000	0.00826000	9.68989000	-1.66635330
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Al	-2.41059000	6.98630000	10.71830000	2.47989170
Al	0.00953000	11.17808000	10.71830000	2.47709580
Al	0.00953000	2.79452000	10.71830000	2.47736150
Al	2.42966000	6.98630000	10.71830000	2.47802490
Al	4.84978000	2.79452000	10.71830000	2.47909610
Al	4.84978000	11.17808000	10.71830000	2.47474310
Al	7.26991000	6.98630000	10.71830000	2.47802820
Al	9.69003000	2.79452000	10.71830000	2.47409980
Al	-4.83072000	8.38356000	10.98601000	2.47133320
Al	-2.41059000	4.19178000	10.98601000	2.47157220
Al	0.00953000	8.38356000	10.98601000	2.47158440
Al	0.00954000	0.00000000	10.98601000	2.46951800
Al	2.42966000	4.19178000	10.98601000	2.47302060
Al	4.84978000	0.00000000	10.98601000	2.47444990

Al	4.84978000	8.38356000	10.98601000	2.47364560
Al	7.26991000	4.19178000	10.98601000	2.47197000
Al	9.69003000	0.00000000	10.98601000	2.46934790
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O	3.96195000	7.00491000	11.88678000	-1.59602180
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Al	2.43251000	9.79620000	11.84896000	2.41555210
Al	4.93520000	5.59136000	12.42329000	2.37432010
Al	7.27210000	9.79464000	11.86550000	2.41879270
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Al	12.06180000	1.37996000	11.77906000	2.41208570
Pt	4.96973000	5.84754000	14.97159000	-0.47832600
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C	6.41023000	6.86554000	16.17401000	-0.22452410
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Al	4.84978000	8.38356000	1.70482000	2.46334520
Al	7.26991000	4.19178000	1.70482000	2.46339050
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Al	2.42966000	1.39726000	2.20274000	2.48272580
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Al	2.42966000	1.39726000	6.11030000	2.47594880
Al	2.42966000	9.78082000	6.11030000	2.47650700
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Al	2.42966000	1.39726000	8.78548000	2.47232130
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O	-1.64959000	5.49336000	9.68989000	-1.66164460
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O	0.77054000	1.30159000	9.68989000	-1.65651940
O	0.92195000	4.20004000	9.68989000	-1.66755410
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O	3.19067000	5.49336000	9.68989000	-1.64704080
O	3.34208000	0.00826000	9.68989000	-1.66789480

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O	8.03091000	5.49336000	9.68989000	-1.65942100
O	8.18232000	0.00826000	9.68989000	-1.66502810
O	8.18232000	8.39182000	9.68989000	-1.65542270
O	10.45104000	1.30158000	9.68989000	-1.66003000
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O	13.02257000	0.00826000	9.68989000	-1.65796510
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Al	-2.41059000	6.98630000	10.71830000	2.47661400
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Al	0.00953000	2.79452000	10.71830000	2.47750050
Al	2.42966000	6.98630000	10.71830000	2.47590650
Al	4.84978000	2.79452000	10.71830000	2.47821860
Al	4.84978000	11.17808000	10.71830000	2.47564910
Al	7.26991000	6.98630000	10.71830000	2.47839570
Al	9.69003000	2.79452000	10.71830000	2.47599240
Al	-4.83072000	8.38356000	10.98601000	2.47437000
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Al	0.00954000	0.00000000	10.98601000	2.47300270
Al	2.42966000	4.19178000	10.98601000	2.47302570
Al	4.84978000	0.00000000	10.98601000	2.47088000
Al	4.84978000	8.38356000	10.98601000	2.47426890
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O	6.36125000	11.21925000	11.90905000	-1.57463340
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O	8.80394000	7.05083000	11.86616000	-1.62300320
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Al	7.29110000	9.73489000	12.37924000	2.37664120
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C	3.39180000	3.68044000	15.19875000	-0.22193530
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O	0.75091000	6.87314000	0.85241000	-1.55781760
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Al	4.84978000	0.00000000	1.70482000	2.46327640
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Al	2.42966000	9.78082000	2.20274000	2.48263220
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Al	2.42966000	6.98630000	3.90756000	2.47749950
Al	4.84978000	2.79452000	3.90756000	2.47764860
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Al	2.42966000	1.39726000	6.11030000	2.47626810
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Al	7.26991000	9.78082000	6.11030000	2.47605270
Al	7.26991000	1.39726000	6.11030000	2.47598710
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Al	12.11016000	1.39726000	6.11030000	2.47565740
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O	13.59502000	1.39291000	7.46570000	-1.65413250
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Al	2.42966000	4.19178000	8.32833000	2.46995500
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Al	2.42966000	1.39726000	8.78548000	2.47652310
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O	0.77054000	9.68514000	9.68989000	-1.65634610
O	0.77054000	1.30159000	9.68989000	-1.64907110
O	0.92195000	4.20004000	9.68989000	-1.65773630
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O	8.18232000	0.00826000	9.68989000	-1.66767850
O	8.18232000	8.39182000	9.68989000	-1.66737350
O	10.45104000	1.30158000	9.68989000	-1.66352910
O	10.60245000	4.20004000	9.68989000	-1.66939340
O	13.02257000	0.00826000	9.68989000	-1.66384020
Al	-4.83072000	11.17808000	10.71830000	2.47837650
Al	-2.41059000	6.98630000	10.71830000	2.48049800
Al	0.00953000	11.17808000	10.71830000	2.47817660
Al	0.00953000	2.79452000	10.71830000	2.47738210

Al	2.42966000	6.98630000	10.71830000	2.48170280
Al	4.84978000	2.79452000	10.71830000	2.47912610
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Al	7.26991000	6.98630000	10.71830000	2.48062110
Al	9.69003000	2.79452000	10.71830000	2.47425250
Al	-4.83072000	8.38356000	10.98601000	2.47285770
Al	-2.41059000	4.19178000	10.98601000	2.47051490
Al	0.00953000	8.38356000	10.98601000	2.47328890
Al	0.00954000	0.00000000	10.98601000	2.46973560
Al	2.42966000	4.19178000	10.98601000	2.47185660
Al	4.84978000	0.00000000	10.98601000	2.47245680
Al	4.84978000	8.38356000	10.98601000	2.47098010
Al	7.26991000	4.19178000	10.98601000	2.47358120
Al	9.69003000	0.00000000	10.98601000	2.46961150
O	-5.66017000	12.49122000	11.85448000	-1.60832860
O	-5.54449000	9.82488000	11.85001000	-1.62220250
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O	-0.86620000	7.02463000	11.84939000	-1.61288390
O	-0.81127000	12.47731000	11.85342000	-1.62341290
O	-0.78263000	4.08184000	11.90189000	-1.57264790
O	-0.70380000	9.82503000	11.85128000	-1.62248450
O	-0.73240000	1.45631000	11.87910000	-1.61497780
O	1.51584000	2.83463000	11.87512000	-1.59858770
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O	11.22650000	2.86031000	11.84956000	-1.62516460
Al	-2.41100000	9.77947000	11.89461000	2.41448620
Al	0.02256000	5.62807000	12.38124000	2.38050520

Al	2.40824000	1.36954000	12.34758000	2.36834320
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Al	12.06163000	1.38212000	11.75403000	2.41299530
Pt	-0.14550000	5.23187000	14.86140000	-0.87751190
Pt	2.10771000	1.77919000	14.83826000	-0.99938470
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Pt	5.00620000	5.74700000	14.92069000	-0.52788820
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C	7.18090000	5.77736000	15.05666000	-0.13033990
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H	7.53051000	4.84496000	15.50706000	0.04528940
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